



Theoretical Diagnostics for the Physical Conditions in Active Galactic Nuclei under the View of JWST

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Abstract

With excellent spectral and angular resolutions and, especially, sensitivity, the JWST allows us to observe infrared emission lines that were previously inaccessible or barely accessible. These emission lines are promising for evaluating the physical conditions in different galaxies. Based on MAPPINGS V photoionization models, we systematically analyze the dependence of over 20 mid-infrared (mid-IR) emission lines covered by MIRI on board JWST on the physical conditions of different galactic environments, in particular narrow-line regions in active galactic nuclei (AGN). We find that mid-IR emission lines of highly ionized argon (i.e., [Ar V] 7.90 and 13.10 μm) and neon (i.e., [Ne V] 14.32 and 24.32 μm , and [Ne VI] 7.65 μm) are effective in diagnosing the physical conditions in AGN. We accordingly propose new prescriptions to constrain the ionization parameter (U), peak energy of the AGN spectrum (E_{peak}), metallicity ($12 + \log(\text{O}/\text{H})$), and gas pressure (P/k) in AGN. These new calibrations are applied to the central regions of six Seyfert galaxies included in the Galaxy Activity, Torus, and Outflow Survey as a proof of concept. We also discuss the similarity and difference in the calibrations of these diagnostics in AGN of different luminosities, highlighting the impact of hard X-ray emission and particularly radiative shocks, as well as the different diagnostics in star-forming regions. Finally, we propose diagnostic diagrams involving [Ar V] 7.90 μm and [Ne VI] 7.65 μm to demonstrate the feasibility of using the results of this study to distinguish galactic regions governed by different excitation sources.

Unified Astronomy Thesaurus concepts: Active galactic nuclei (16); Infrared spectroscopy (2285); Interstellar line emission (844); James Webb Space Telescope (2291); Photoionization (2060); Shocks (2086)

Materials only available in the online version of record: machine-readable tables

1. Introduction

Supermassive black holes reside in most, if not all, massive galaxies and up to $\sim 40\%$ of the black holes in emission-line

galaxies manifest as active galactic nuclei (AGN; i.e., G. Kauffmann et al. 2003; C. J. Miller et al. 2003; and see review L. C. Ho 2008). A growing body of evidence has revealed that AGN play an important role in determining the evolutionary pathways and final fate of galaxies through different modes of feedback processes (e.g., T. Di Matteo et al. 2005; P. F. Hopkins et al. 2008; R. Weinberger et al. 2017; R. Davé et al. 2019; and see the reviews by B. R. McNamara & P. E. J. Nulsen 2007; A. C. Fabian 2012; C. M. Harrison &

C. Ramos Almeida 2024). The electromagnetic spectrum of a galaxy contains a wealth of information on the fundamental physical conditions contributing to the recurrent feedback processes (see the reviews by P. Padovani et al. 2017; L. J. Kewley et al. 2019; A. Sajina et al. 2022). In this regard, theoretical photoionization modeling plays a crucial role in interpreting observed AGN spectra, and thus using observations to constrain the physical conditions in AGN for a comprehensive understanding of galaxy evolution.

AGN photoionization modeling has been developed for over a half century from the early calculations of quasars and X-ray nebulae (e.g., G. R. Burbidge et al. 1966; D. E. Osterbrock & R. A. R. Parker 1966; C. B. Tarter & E. E. Salpeter 1969; C. B. Tarter et al. 1969; see the review by L. J. Kewley et al. 2019). During this period, two large photoionization codes (i.e., MAPPINGS and CLOUDY) gradually developed into the most commonly used codes for photoionization modeling. Specifically, both MAPPINGS and CLOUDY include self-consistent treatment of nebular and dust physics with different atomic data sets and calculation methods. In addition, MAPPINGS includes radiative shock physics (R. S. Sutherland & M. A. Dopita 1993, 2017), while CLOUDY includes molecular physics (G. J. Ferland et al. 1998; M. Chatzikos et al. 2023). Therefore, MAPPINGS can be applied to H II regions, AGN, and shocked regions, while CLOUDY can be applied to H II regions, AGN, and photodissociation regions. Despite their differences, the theoretical AGN photoionization models calculated by MAPPINGS and CLOUDY with the same inputs present similar correlations between emission-line ratios, gas metallicity, and ionization parameter (P. Zhu et al. 2023).

Among key parameters of theoretical photoionization modeling, the effect of different metallicities on the predicted emission-line ratios has been extensively studied for the direct calibration of metallicity in star-forming (SF) galaxies, as well as in AGN (e.g., T. Nagao et al. 2011; M. Pereira-Santaella et al. 2017; L. J. Kewley et al. 2019; B. Pérez-Díaz et al. 2022; M. Martínez-Paredes et al. 2023; P. Zhu et al. 2024, and references therein). The effect of another key parameter, the ionization parameter (U), commonly defined as the ratio of the number density of incident ionizing photons (Φ) and the number density of hydrogen atoms (n_{H}) multiplied by the speed of light ($U = \frac{\Phi}{c n_{\text{H}}}$ where $\Phi = \frac{\int_{\nu_0}^{\infty} L_{\nu} d\nu / h\nu}{4\pi r^2}$), has been also considered in the above studies to better constrain the calibration of metallicity. However, an accurate calibration of the ionization parameter U itself, especially in AGN, is still lacking. U is an important parameter determined together by the spectral energy distribution (SED) of the ionizing radiation field, the gas density, and the distance of the ionized gas relative to the ionizing source. Variations in U shed important light on underlying evolutionary processes in galaxies at different redshifts (e.g., N. P. Abel et al. 2009; R. L. Sanders et al. 2016; D. Kashino & A. K. Inoue 2019; N. A. Reddy et al. 2023).

More specifically, measurements of the ionization parameter in AGN can also be used to help quantify gas outflow rates (e.g., D. Baron & H. Netzer 2019; R. Davies et al. 2020), as well as help decode the feedback effects responsible for observations such as, but not limited to, the unique characteristics of polycyclic aromatic hydrocarbon (PAH) emission (e.g., O. V. Egorov et al. 2023; I. García-Bernete et al. 2024b; L. Zhang et al. 2024a) in AGN. Empirical calibrations of U can be achieved using any paired lines with different dependences on U of their emissivities (which are intrinsically dependent on

electron density and temperature). JWST spectral observations provide access to study a variety of infrared emission lines covering a wide range of critical densities and ionization potentials (IPs; e.g., M. Pereira-Santaella et al. 2022, 2024; L. Armus et al. 2023; K. Goold et al. 2024; L. Zhang et al. 2024b; A. Alonso Herrero et al. 2025; V. Buiten et al. 2025; M. Ceci et al. 2025; L. Hermosa Muñoz et al. 2025; C. Marconcini et al. 2025; P. M. Ogle et al. 2025; C. Ramos Almeida et al. 2025). Most of these emission lines were barely available in the past due to the limited spectral resolution and/or sensitivity of previous instruments such as spectrographs on board the Infrared Space Observatory and Spitzer Space Telescope (Spitzer). Thus, we now have an unprecedented opportunity to explore in depth and fully utilize infrared emission lines detected in AGN with JWST to evaluate the effect of the ionization parameter in diagnostic diagrams.

This paper aims to explore the theoretical dependence of the mid-infrared (mid-IR) fine structure emission-line ratios on the physical conditions of AGN, in particular the ionization parameter, and complementarily, the E_{peak} , metallicity, and gas pressure, which are also important physical parameters in AGN. This study can provide a more comprehensive explanation for JWST observations, thereby further advancing the analysis of future observational work. Specifically, we focus on mid-IR emission lines accessible by the Medium Resolution Spectrograph (MRS; M. Wells et al. 2015; A. Labiano et al. 2021; I. Argyriou et al. 2023) on the Mid-Infrared Instrument (MIRI; G. H. Rieke et al. 2015; G. S. Wright et al. 2015, 2023) of JWST (J. P. Gardner et al. 2023; J. Rigby et al. 2023). The near-IR ($\sim 1\text{--}5 \mu\text{m}$) spectra of galaxies, although covering some weak coronal lines, are mainly composed of emission lines from hydrogen, helium, and iron and are not considered here.

This paper is structured as follows. After introducing the adopted theoretical models (Section 2), we elaborate on the calibration of U and propose some optimal prescriptions according to a feature extraction method based on the Pearson correlation coefficient combining some practical criteria (Section 3.1). The following sections discuss the calibrations of E_{peak} (Section 3.2), metallicity (Section 3.3), and gas pressure (Section 3.4), as well as the application of these calibrations in observed AGN (Section 3.5). In addition, we discuss the calibrations in low-luminosity AGN (Section 4.1), highlighting the effect of hard X-ray radiation (Section 4.1.1) and potential shocks (Section 4.1.2). Section 4 also discusses the different calibrations in star-forming (SF) regions (Section 4.2) and the potential application of the above results in future studies of distinguishing galactic regions governed by different excitation sources (Section 4.3). A summary of the main results of this paper is provided in Section 5.

2. Theoretical Models

As mentioned in the introduction section, the two most popular codes for photoionization modeling are MAPPINGS and CLOUDY, which are implemented independently with self-consistent atomic data and physical processes (R. S. Sutherland & M. A. Dopita 1993; G. J. Ferland et al. 1998; R. S. Sutherland & M. A. Dopita 2017; M. Chatzikos et al. 2023). Specifically, MAPPINGS can be applied to H II regions, AGN, and shocked regions, while CLOUDY can be applied to H II regions, AGN, and photodissociation regions. Overall, the theoretical AGN photoionization models calculated by the two codes provide similar predictions when using the same inputs, with most of the predicted emission-

line ratios agreeing to within 0.1 dex (P. Zhu et al. 2023). The existing discrepancy is mainly due to the difference in the implementation of inherent physical processes and the adopted atomic data sets. Since this paper requires theoretical models for shocked regions without attempting to model the photodissociation regions, all theoretical models presented in the following sections are calculated using MAPPINGS.

We use the latest version (5.21) MAPPINGS V²⁴ code to model the interstellar medium (ISM) in the narrow-line regions (NLRs) surrounding the AGN. The latest available atomic data from CHIANTI version 10 (G. Del Zanna et al. 2021) is included in MAPPINGS V. For the theoretical AGN photoionization models, we adopt realistic SEDs derived by the AGN radiation model OPTXAGNF²⁵ as the incident ionizing radiation sources (C. Done et al. 2012; C. Jin et al. 2012). The adopted AGN radiation sources include soft X-ray excess with energy between ~ 0.2 and 2 keV, which can be important for the excitation of infrared forbidden lines. To model various types of AGN, we sample the black hole masses (from 10^6 to $10^9 M_\odot$) and Eddington ratios (from 10^{-5} to 1) both in increments of 0.5 dex as input to the embedded OPTXAGNF in MAPPINGS V. The black hole mass and Eddington ratio together contribute to a shift of the peak energy, i.e., E_{peak} , of the AGN spectrum as described by Equations (4)–(6) in A. D. Thomas et al. (2016, see also FigurA13 therein). Other parameters of OPTXAGNF are set to be the recommended values²⁶ for NLRs in MAPPINGS V (see Figure 1 for examples of the AGN ionizing radiation sources). Potential caveats of the adopted AGN SEDs are discussed in Section 4.1.

For each AGN photoionization model, we adopt the abundance scaling relations provided by D. C. Nicholls et al. (2017) and consider the metallicity variation from $12 + \log(\text{O}/\text{H}) = 8.150, 8.427, 8.632, 8.760, 8.850, 8.943, \text{ to } 8.997$ (i.e., 0.2, 0.4, 0.7, 1.0, 1.3, 1.7, and 2.0 Z_\odot). The adopted abundance scaling relations applied a more realistic cosmic abundance standard (M.-F. Nieva & N. Przybilla 2012), instead of a solar abundance standard. Dust depletion effect, an important factor in ensuring reliable models in high-metallicity regions (P. Zhu et al. 2023), is included in the model with the depletion factors derived by A. D. Thomas et al. (2018) according to the results of E. B. Jenkins (2009). We adopt a plane-parallel geometry in the AGN photoionization modeling with the ionization parameter $\log U$ at the inner edge of the cloud varying from -4.8 to -1.3 with a 0.5 dex step size.²⁷ Furthermore, we adopt an isobaric structure in the calculation, with the gas pressure $\log(P/k)$ varying from 5.5 to 8.5, unless specifically noted, with a 0.5 dex step size. An isochoric structure can be selected as well, while the model results based on these two structures do not change much in terms of the line ratio predictions (e.g., M. Pereira-Santaella et al. 2010, 2017, 2024; T. Nagao et al. 2011). The detailed calculation of the AGN model proceeds at a 2% photon absorption step and stops when the hydrogen becomes 99% neutral (with an N_{H} of $\sim 10^{21}$ – 10^{22} cm^{-2}). The model results calculated using the different models involved in this paper are available in the Appendix.

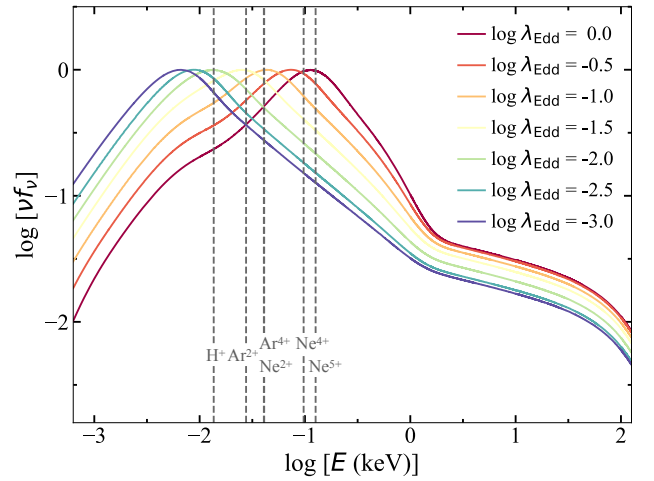


Figure 1. Examples of the AGN ionizing spectra calculated by OPTXAGNF for AGN photoionization models with the black hole mass set as $10^7 M_\odot$ and the Eddington ratio (i.e., λ_{Edd}) ranging from 10^{-3} to 1. The vertical lines indicate the required ionization energies of marked ions. All AGN ionizing spectra are normalized by the peak flux for illustration. Note that the energy corresponding to the peak flux (i.e., E_{peak} , in units of keV) increases along with an increase of λ_{Edd} and a decrease of black hole mass.

Table 1
Basic Information of the Selected Emission Lines

Line	λ (μm)	IP (eV)	$\log n_c$ (cm^{-3})
(1)	(2)	(3)	(4)
[Fe II]	5.34	7.9	2.48
[Fe VIII]	5.45	124	...
[Mg VII]	5.50	186.5	6.53
[Mg V]	5.61	109.2	6.60
[Ar II]	6.99	15.8	5.62
[Na III]	7.32	47.3	...
Pf α	7.46	13.6	...
[Ne VI]	7.65	126.2	5.80
[Fe VII]	7.82	99.1	6.10
[Ar V]	7.90	40.7	5.20
[Ar III]	8.99	27.6	5.28
[Fe VII]	9.53	99.1	5.74
[S IV]	10.51	34.8	4.75
Hu α	12.37	13.6	...
[Ne II]	12.81	21.6	5.80
[Ar V]	13.10	40.7	4.47
[Ne V]	14.32	97.1	4.51
[Ne III]	15.56	40.1	5.32
[S III]	18.71	23.3	4.08
[Ar III]	21.83	27.6	5.38
[Ne V]	24.32	97.1	3.77
[O IV]	25.89	54.9	4.00
[Fe II]	25.99	7.9	4.11

Note. Column (1): line name. Column (2): rest wavelength. Column (3): IP. Column (4): critical electron density for collisional excitation calculated by PYNEB (V. Luridiana et al. 2015) at $T_e = 10^4 \text{ K}$.

3. Modeling Results and Applications

The primary goal of this work is to extract the optimal line ratio diagnostics accessible by JWST/MRS spectral observations to quantify the ionization parameter (i.e., U) in AGN for science goals as exemplified in the introduction section. We are also interested in diagnostics of the hardness of ionizing radiation field (i.e., E_{peak}), metallicity, and gas pressure in

²⁴ <https://mappings.anu.edu.au/>

²⁵ <https://heasarc.gsfc.nasa.gov/xanadu/xspec/manual/node211.html>

²⁶ $a_s = 0$, $r_{\text{cor}} = 40 R_g$, $r_{\text{out}} = 10^4 R_g$, $kT_c = 0.2 \text{ keV}$, $\tau = 15$, $\Gamma = 2.2$, and $f_{\text{pl}} = 0.2$.

²⁷ The $\log U$ values already include the systematic differences in the definitions from the values calculated using spherical geometry models and can therefore be directly compared with them.

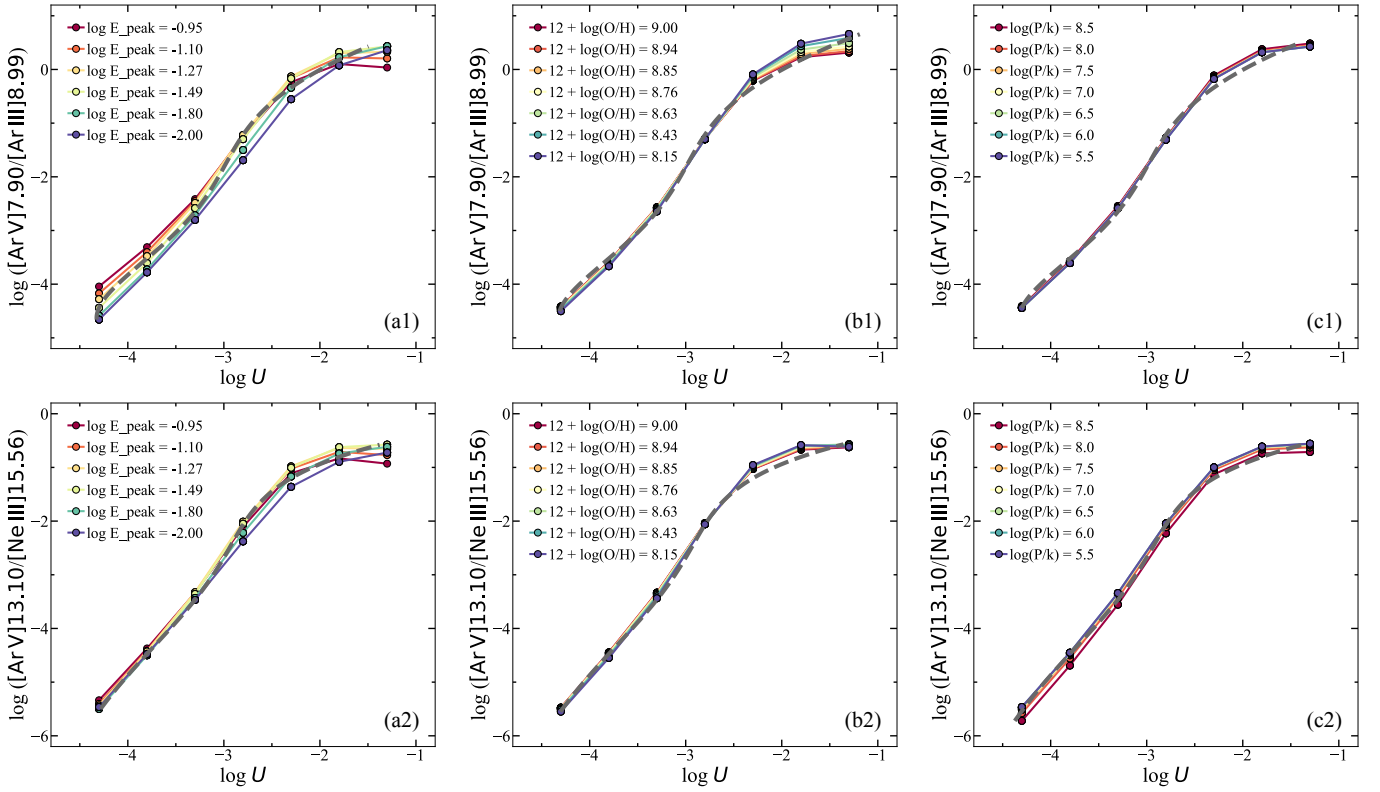


Figure 2. Dependence of (top) $[\text{Ar V}] 7.90 \mu\text{m}/[\text{Ar III}] 8.99 \mu\text{m}$ and (bottom) $[\text{Ar V}] 13.10 \mu\text{m}/[\text{Ne III}] 15.56 \mu\text{m}$ on the ionization parameter (U), as predicted by AGN photoionization models (colored points). Each panel displays model results under specific parameter constraints: (a1 and a2) $12 + \log(\text{O}/\text{H}) = 8.76$ and $\log(P/k) = 7.0$; (b1 and b2) $\log E_{\text{peak}} = -1.49$ and $\log(P/k) = 7.0$; and (c1 and c2) $\log E_{\text{peak}} = -1.49$ and $12 + \log(\text{O}/\text{H}) = 8.76$, while the gray dashed line represents the best-fit correlation (Equation (1)) derived from all AGN models in Section 3.

AGN, as these parameters play important roles in determining the physical conditions and hence corresponding evolutionary processes therein.

To this end, we first select 23 sufficiently strong lines (overall $\gtrsim 0.1\%$ of $\text{H}\beta$ emission) within JWST/MRS bands based on their line strengths predicted by the theoretical AGN models in order to analyze their dependence on the physical conditions of AGN (see Table 1 for the emission-line list and Table A1 for the modeling results). We confirm that these selected lines are all detectable with JWST/MRS according to recent studies of nearby Seyferts (e.g., M. Pereira-Santaella et al. 2022; L. Armus et al. 2023; L. Zhang et al. 2024b; A. Alonso-Herrero et al. 2025; M. Ceci et al. 2025; L. Hermosa Muñoz et al. 2025; C. Marconcini et al. 2025). The only exception is the $[\text{Fe II}] 25.99 \mu\text{m}$ emission line, which was not reported in all of the observations, especially for the nuclear regions. The lack of $[\text{Fe II}] 25.99 \mu\text{m}$ emission is likely because most Fe^+ are in high level populations (corresponding to stronger $[\text{Fe II}] 5.34 \mu\text{m}$ emission) in the hot environments adjacent to AGN, or simply due to the sensitivity issue of MRS Channel 4 observations. All combinations of any two lines in Table 1 are under consideration for the selection of the optimal diagnostics.

3.1. Ionization Parameter Diagnostics

To efficiently extract the optimal U diagnostics, we use a feature extraction method based on the Pearson correlation coefficient.²⁸ Specifically, for all combinations of any two

lines in Table 1, we first calculate the Pearson correlation coefficient between the logarithmic line ratio and $\log U$ of the theoretical AGN models. All line ratios are then ranked according to the absolute values of their corresponding Pearson correlation coefficients. As an additional quality control check, we visually inspect each correlation between the logarithmic line ratios and $\log U$, from the correlations with high to low absolute Pearson correlation coefficients. Overall, line ratios involving $[\text{Ar V}]$ work the best as U diagnostics, followed by line ratios involving $[\text{Ne V}]$, and finally line ratios involving $[\text{O IV}]$ with larger scatter. This result indicates that the $[\text{Ar V}]$ emissivity has the strongest dependence on U .

Considering that $[\text{Ar V}]$ has the best performance in U diagnostics, we then combine some practical criteria to select the optimal U diagnostics from the line ratios involving $[\text{Ar V}]$. Specifically, we first consider the line ratios of paired lines with close wavelengths to better avoid the influence of dust extinction in observations (even if relatively small in the mid-IR). Moreover, the line ratios of paired lines close in wavelengths falling in the same JWST/MRS channel are also more time efficient to be observed. Second, when given the comparable robustness, we prefer the line ratios of paired lines with shorter wavelengths, since shorter wavelengths correspond to higher spatial and spectral resolutions in JWST observations, and are applicable to a wider redshift range. Based on the result of the feature extraction process and these practical criteria, Figure 2 demonstrates two optimal U diagnostics (i.e., $[\text{Ar V}] 7.90 \mu\text{m}/[\text{Ar III}] 8.99 \mu\text{m}$, and $[\text{Ar V}] 13.10 \mu\text{m}/[\text{Ne III}] 15.56 \mu\text{m}$). Besides the tight

²⁸ The Pearson correlation coefficient measures the linear correlation between two variables and it is essentially a normalized measurement of the covariance. Its value lies between -1 and $+1$, where -1 and $+1$ indicate ideal negative and positive linear correlations, respectively.

correlations, the two U diagnostics also have their own pros and cons.

The line ratio $[\text{Ar V}] 7.90 \mu\text{m}/[\text{Ar III}] 8.99 \mu\text{m}$ best follows the practical criteria as discussed, but it has a slightly secondary dependence on E_{peak} due to the different IPs of $[\text{Ar V}]$ and $[\text{Ar III}]$. The line ratio $[\text{Ar V}] 13.10 \mu\text{m}/[\text{Ne III}] 15.56 \mu\text{m}$ is relatively less sensitive to E_{peak} given the similar IPs of $[\text{Ar V}]$ and $[\text{Ne III}]$. However, this line ratio has a slight dependence on gas pressure due to the different critical densities of $[\text{Ar V}] 13.10 \mu\text{m}$ and $[\text{Ne III}] 15.56 \mu\text{m}$ and this line ratio falls in longer-wavelength MRS band. Nevertheless, these two line ratios, considering the tight correlations as shown in Figure 2, remain numerically (and physically; see Section 4.1.1) the best diagnostics for U , especially when compared to line ratio diagnostics for U in AGN based on relatively low ionization lines (e.g., M. Pereira-Santaella et al. 2017; P. Zhu et al. 2024). An alternative U diagnostic is $[\text{Ar V}] 7.90 \mu\text{m}/[\text{Ne III}] 15.56 \mu\text{m}$, which has even weaker dependence on both E_{peak} and gas pressure given the comparable IPs and critical densities of $[\text{Ar V}] 7.90 \mu\text{m}$ and $[\text{Ne III}] 15.56 \mu\text{m}$, whereas this line ratio is not the best in observations considering their significantly separate wavelengths. This line ratio might be in turn used to constrain different dust extinction models with known U .

To calibrate U with these line ratios, we adopt a quintic function, i.e., Equation (1):

$$\begin{aligned} \log U = & c_5 \times (\log R)^5 + c_4 \times (\log R)^4 \\ & + c_3 \times (\log R)^3 \\ & + c_2 \times (\log R)^2 + c_1 \times \log R + c_0, \end{aligned} \quad (1)$$

and perform a least squares fit of the curved correlations between the input $\log U$ and predicted line ratios using the Levenberg–Marquardt algorithm. Note that we selected the quintic function (as well as other functions adopted in the following subsections) from among different functions simply because they can provide numerically accurate calibrations for the model results studied here, and the functions adopted in other specific studies may differ.

The best-fit coefficients for $R = [\text{Ar V}] 7.90 \mu\text{m}/[\text{Ar III}] 8.99 \mu\text{m}$, $[\text{Ar V}] 13.10 \mu\text{m}/[\text{Ne III}] 15.56 \mu\text{m}$, and also $[\text{Ar V}] 7.90 \mu\text{m}/[\text{Ne III}] 15.56 \mu\text{m}$, are listed in the Appendix. As a quantification for the robustness of the quintic function fitting, we calculate the rms scatter of the best-fit correlations relative to the model results, which are 0.16 dex and 0.17 dex for $[\text{Ar V}] 7.90 \mu\text{m}/[\text{Ar III}] 8.99 \mu\text{m}$ and $[\text{Ar V}] 13.10 \mu\text{m}/[\text{Ne III}] 15.56 \mu\text{m}$, respectively. The best-fit correlations in this section are all for AGN models with relatively high E_{peak} as illustrated in Figure 2(a). The best-fit results for AGN models with low E_{peak} (namely low-luminosity AGN) are specifically discussed in Section 4 given the bivaluation dependence of the predicted line ratios on E_{peak} . In fact, since the line ratio diagnostics of U have basically no dependence on E_{peak} , the best-fit results for different E_{peak} ranges are essentially the same.

3.2. Peak Energy Diagnostics

As illustrated in Figure 1, the energy corresponding to the peak flux (i.e., E_{peak} , in keV units) of the AGN ionizing spectrum increases along with an increase of λ_{Edd} . Higher E_{peak} of the AGN ionizing spectrum with relatively more high-energy ionizing photons essentially corresponds to harder

radiation fields in AGN. Therefore, in the following discussion, we use the radiation field hardness in AGN synonymously with E_{peak} . Variations in radiation field hardness and the corresponding line ratio diagnostics in observations are critical to constrain theoretical models (e.g., D. Rigopoulou et al. 1996; M. D. Thornley et al. 2000; U. Giveon et al. 2002; A. Verma et al. 2003; B. T. Draine et al. 2021) and to explain observational ISM properties of different galaxies (e.g., R. Genzel et al. 1998; E. Sturm et al. 2002; L. K. Hunt et al. 2010; E. Pérez-Montero et al. 2024, 2025; D. Baron et al. 2025). The ratios of mid-IR emission lines from the same element but of different excitation levels (e.g., $[\text{Ne V}] 14.32 \mu\text{m}/[\text{Ne II}] 12.81 \mu\text{m}$, $[\text{Ne III}] 15.56 \mu\text{m}/[\text{Ne II}] 12.81 \mu\text{m}$, $[\text{Ar III}] 8.99 \mu\text{m}/[\text{Ar II}] 6.99 \mu\text{m}$, and $[\text{S IV}] 10.51 \mu\text{m}/[\text{S III}] 18.71 \mu\text{m}$) have long been proposed to be good diagnostics of the ionizing radiation field hardness (e.g., R. Genzel et al. 1998; M. D. Thornley et al. 2000; U. Giveon et al. 2002; A. Verma et al. 2003). The ratios of some UV/optical emission lines (e.g., $\text{He II } \lambda 1640/\text{He I } \lambda 3187$, $\text{He II } \lambda 1640/\text{H}\beta$, and $[\text{He II}] \lambda 4686/\text{H}\beta$) have also been recently proposed to have the same function (P. Zhu et al. 2024).

In principle, the optimal E_{peak} diagnostics of AGN within JWST/MRS bands are those line ratios involving the infrared lines of very high IPs (e.g., $[\text{Ne VI}] 7.65 \mu\text{m}$, $[\text{Fe VIII}] 5.45 \mu\text{m}$, and $[\text{Mg V}] 5.61 \mu\text{m}$ with IP > 100 eV). These high-IP lines have several advantages in diagnosing E_{peak} in AGN. First, these lines can only be produced in regions with very high-energy photons and are hence more sensitive to the variation of the peak energy of AGN ionizing radiation field. Moreover, these high-IP lines can barely be produced by starbursts, which can contribute significantly to the excitation of the relatively low-IP lines such as $[\text{Ne III}] 15.56 \mu\text{m}$, $[\text{Ar III}] 8.99 \mu\text{m}$, and $[\text{S IV}] 10.51 \mu\text{m}$ (see Section 4.2). We noted that $[\text{Ne V}] 14.32 \mu\text{m}$ and $[\text{Ne VI}] 7.65 \mu\text{m}$ have been recently detected using JWST/MIRI observations in the nuclear region of M83, previously known as a purely starburst system, but such detection are still more likely due to excitation of fast radiative shocks or weakly accreting AGN rather than starbursts (i.e., S. Hernandez et al. 2025). These lines are also less affected by dust extinction than the UV–optical diagnostics. We therefore expect that these infrared lines of very high IPs will be more widely used in diagnosing the radiation field hardness in the era of JWST.

Applying the same feature extraction process as detailed in Section 3.1, we find that none of the line ratios works as effectively in directly diagnosing E_{peak} as in diagnosing U . Some line ratios investigated here do have a secondary dependence on E_{peak} , but still with a primary dependence on U . We therefore adopt a different strategy for the calibration of E_{peak} as described by Equation (2):

$$\log E_{\text{peak}} = a \times (\log R - b)^2 + c, \quad (2)$$

where

$$\begin{aligned} a = & a_{z,2} \times (12 + \log(\text{O}/\text{H}))^2 \\ & + a_{z,1} \times (12 + \log(\text{O}/\text{H})) \\ & + a_{u,1} \times \log U + a_0, \end{aligned} \quad (3)$$

$$\begin{aligned} b = & b_{z,2} \times (12 + \log(\text{O}/\text{H}))^2 \\ & + b_{z,1} \times (12 + \log(\text{O}/\text{H})) \\ & + b_{u,1} \times \log U + b_0, \end{aligned} \quad (4)$$

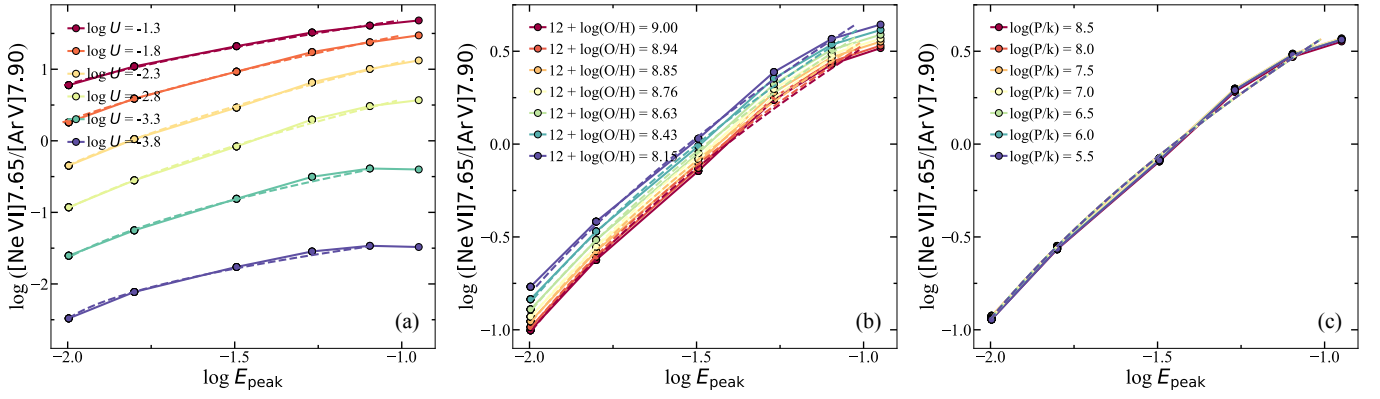


Figure 3. Dependence of $[\text{Ne VI}] 7.65 \mu\text{m}/[\text{Ar V}] 7.90 \mu\text{m}$ on the input AGN spectrum peak energy (E_{peak} , in keV), as predicted by AGN photoionization models (colored points). Each panel displays model results under specific parameter constraints: (a) $12 + \log(\text{O}/\text{H}) = 8.76$ and $\log(P/k) = 7$; (b) $\log U = -2.8$ and $\log(P/k) = 7$; and (c) $\log U = -2.8$ and $12 + \log(\text{O}/\text{H}) = 8.76$. The dashed lines represent the best-fit correlations (Equations (2)–(5)) derived from all AGN models with the given $\log U$ and $12 + \log(\text{O}/\text{H})$.

$$c = c_{Z,2} \times (12 + \log(\text{O}/\text{H}))^2 + c_{Z,1} \times (12 + \log(\text{O}/\text{H})) + c_{U,1} \times \log U + c_0. \quad (5)$$

The prerequisites of this prescription are measurements of the ionization parameter, which can be estimated as discussed above, and metallicity, which can also be constrained using the infrared-line ratios as detailed in Section 3.3.

Following the strategy in Equations (2)–(5), we examined the predicted dependence of all the line ratios involving high-IP lines on E_{peak} and found that the one composed of emission lines from two noble gases, $[\text{Ne VI}] 7.65 \mu\text{m}/[\text{Ar V}] 7.90 \mu\text{m}$, is the best among other emission-line ratios within JWST/MRS bands in diagnosing E_{peak} in AGN (see Figure 3). This result is consistent with the expectation for the high-IP lines in diagnosing E_{peak} in AGN. For any value of $\log U$ between -3.8 and -1.3 , the increase in $[\text{Ne VI}] 7.65 \mu\text{m}/[\text{Ar V}] 7.90 \mu\text{m}$ exceeds 1 dex as $\log E_{\text{peak}}$ changes from -2.0 to -1.0 . Accurate calibrations of $\log U$ values are available as discussed in Section 3.1, and the scatter of $[\text{Ne VI}] 7.65 \mu\text{m}/[\text{Ar V}] 7.90 \mu\text{m}$ due to variations in metallicity remains within 0.30 dex at the low end and 0.15 dex at the high end of $\log E_{\text{peak}}$.

$[\text{Ne VI}] 7.65 \mu\text{m}/[\text{Ar V}] 7.90 \mu\text{m}$ follows the same practical criteria applied to the U diagnostics. The best-fit coefficients in Equation (2) for $R = [\text{Ne VI}] 7.65 \mu\text{m}/[\text{Ar V}] 7.90 \mu\text{m}$ in terms of different U ranges are listed in Table A5. The rms scatter of the piecewise fitting correlations relative to the model results ranges from 0.02 to 0.05 dex. Possible alternative E_{peak} diagnostics in theory are $[\text{Fe VIII}] 5.45 \mu\text{m}/[\text{Mg V}] 5.61 \mu\text{m}$ and $[\text{Mg V}] 5.61 \mu\text{m}/[\text{Fe VII}] 7.82 \mu\text{m}$. However, their diagnostic reliability is greatly undermined in observations due to the significant dust depletion, which can be up to $\sim 99\%$, of iron and magnesium in galaxies. The complex and inhomogeneous extinction due to dirty water ice in the $5.5\text{--}7.5 \mu\text{m}$ band (e.g., I. García-Bernete et al. 2024a) can also complicate the application of these two line ratios in diagnosing E_{peak} .

3.3. Metallicity Diagnostics

Following the traditional definition of metallicity, we first study the feasibility of the relative intensities of infrared neon and argon emission to ionized hydrogen emission (i.e., $\text{Pf}\alpha$

here, the strongest ionized hydrogen line within MIRI/MRS bands) in estimating metallicity. After visually inspecting all such correlations, we find that the high-excitation lines from neon and argon (i.e., $[\text{Ne V}]$, and $[\text{Ar V}]$) are better than the relatively low-excitation lines (i.e., $[\text{Ne III}]$, $[\text{Ne II}]$, $[\text{Ar III}]$, and $[\text{Ar II}]$) in diagnosing metallicity in AGN, although all lines show a primary dependence on U and a weak dependence on E_{peak} . The better performance of the highly excited lines is within expectation given their enhanced emissivities in AGN, i.e., higher sensitivities to the radiation field with varying metallicity. Meanwhile, $[\text{Ar V}]$ emission lines, especially $[\text{Ar V}] 7.90 \mu\text{m}$, correlate better than $[\text{Ne V}]$ emission lines, as $[\text{Ar V}]$ emission lines have much higher critical densities and are therefore not dependent on gas pressure.

We further find that the addition of $[\text{Ar III}] 8.99 \mu\text{m}$ eliminates most of the dependence of $[\text{Ar V}] 7.90 \mu\text{m}$ on E_{peak} . Moreover, the addition of $[\text{Ar III}] 8.99 \mu\text{m}$ mitigates the contamination effect of potential nuclear starbursts in AGN as nuclear starbursts contribute to both the $[\text{Ar III}] 8.99 \mu\text{m}$ and $\text{Pf}\alpha$ emission and hence to a certain degree cancel the contamination effect. We therefore propose an optimal prescription in estimating metallicity with $R = ([\text{Ar III}] 8.99 \mu\text{m} + [\text{Ar V}] 7.90 \mu\text{m})/\text{Pf}\alpha$ (see Figure 4). For any value of $\log U$ between -4.3 and -1.3 , the increase in $([\text{Ar III}] 8.99 \mu\text{m} + [\text{Ar V}] 7.90 \mu\text{m})/\text{Pf}\alpha$ is of 0.7 dex as the metallicity changes from 0.2 to $2.0 Z_{\odot}$. Accurate $\log U$ estimates are available as discussed in Section 3.1, and the scatter of $([\text{Ar III}] 8.99 \mu\text{m} + [\text{Ar V}] 7.90 \mu\text{m})/\text{Pf}\alpha$ due to variations in $\log E_{\text{peak}}$ ranges from 0.01 to 0.17 dex for different $\log U$ values.

Similar to the calibration of E_{peak} , we adopt the strategy as described by Equation (6) to calibrate metallicity in AGN, but with different coefficients:

$$12 + \log(\text{O}/\text{H}) = a \times (\log R - b)^2 + c, \quad (6)$$

where

$$a = a_{E,3} \times (\log E_{\text{peak}})^3 + a_{E,2} \times (\log E_{\text{peak}})^2 + a_{E,1} \times \log E_{\text{peak}} + a_{U,1} \times \log U + a_0, \quad (7)$$

$$b = b_{E,3} \times (\log E_{\text{peak}})^3 + b_{E,2} \times (\log E_{\text{peak}})^2 + b_{E,1} \times \log E_{\text{peak}} + b_{U,1} \times \log U + b_0, \quad (8)$$

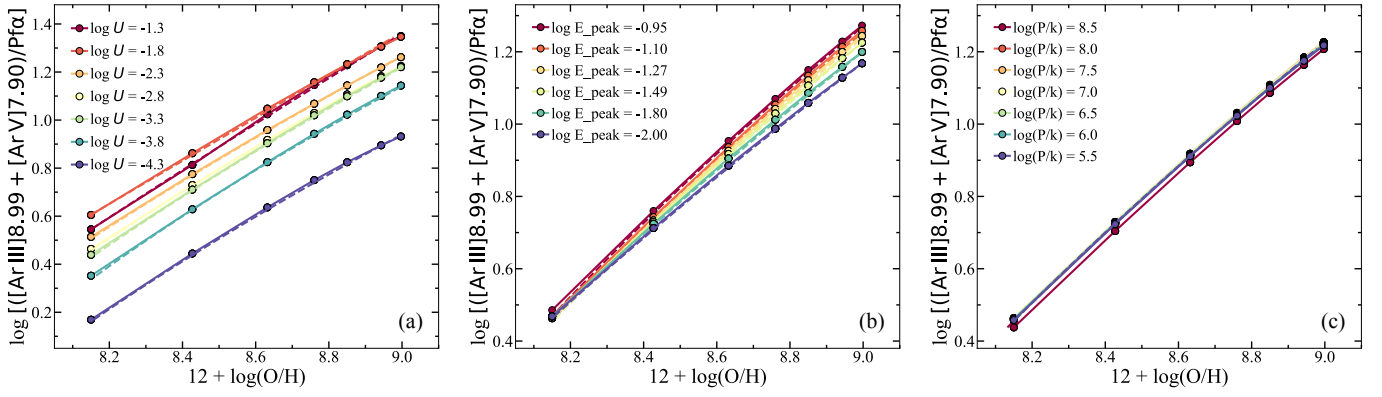


Figure 4. Dependence of $([\text{Ar III}] 8.99 \mu\text{m} + [\text{Ar V}] 7.90 \mu\text{m})/\text{Pf}\alpha$ on the metallicity ($12 + \log(\text{O}/\text{H})$), as predicted by AGN photoionization models (colored points). Each panel displays model results under specific parameter constraints: (a) $\log E_{\text{peak}} = -1.49$ and $\log(P/k) = 7.0$; (b) $\log U = -2.8$ and $\log(P/k) = 7.0$; and (c) $\log U = -2.8$ and $\log E_{\text{peak}} = -1.49$. The dashed lines represent the best-fit correlations (Equations (6)–(9)) derived from all AGN models with the given $\log U$ and $\log E_{\text{peak}}$.

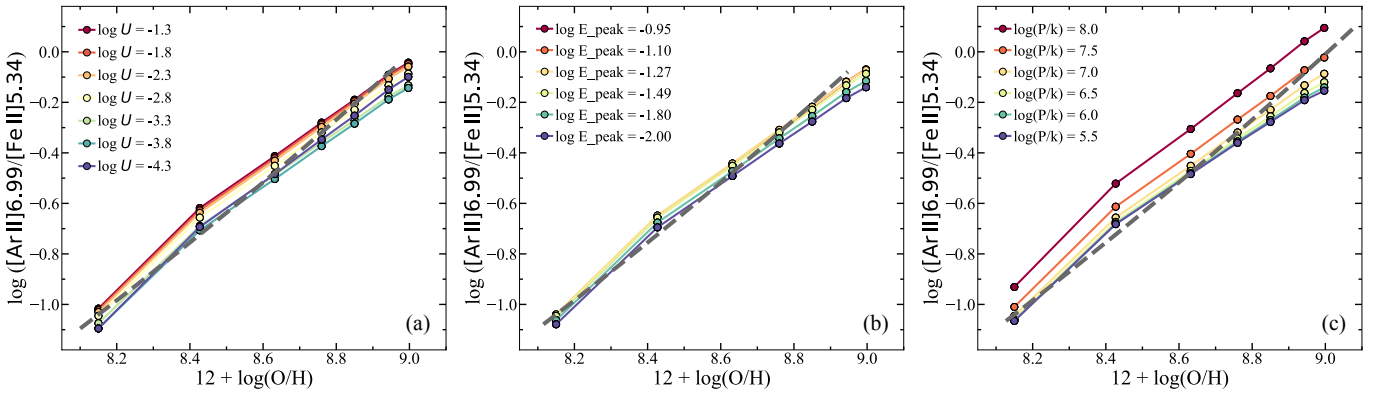


Figure 5. Dependence of $[\text{Ar II}] 6.99 \mu\text{m}/[\text{Fe II}] 5.34 \mu\text{m}$ on the metallicity ($12 + \log(\text{O}/\text{H})$), as predicted by AGN photoionization models (colored points). Each panel displays model results under specific parameter constraints: (a) $\log E_{\text{peak}} = -1.49$ and $\log(P/k) = 7.0$; (b) $\log U = -2.8$ and $\log(P/k) = 7.0$; and (c) $\log U = -2.8$ and $\log E_{\text{peak}} = -1.49$, while the gray dashed line represents the best-fit correlation (Equation (10)) derived from all AGN models with $(P/k) \leq 8.0$.

$$c = c_{E,3} \times (\log E_{\text{peak}})^3 + c_{E,2} \times (\log E_{\text{peak}})^2 + c_{E,1} \times \log E_{\text{peak}} + c_{U,1} \times \log U + c_0. \quad (9)$$

For the above calibration, we do not need to estimate the ionization correction factors as in previous metallicity calibration studies (e.g., N. L. Martín-Hernández et al. 2002; A. Verma et al. 2003; T. Nagao et al. 2011), because the intrinsic parameters that determine the ionization correction factors are already included in the calibration. The best-fit coefficients for the metallicity calibration with $R = ([\text{Ar III}] 8.99 \mu\text{m} + [\text{Ar V}] 7.90 \mu\text{m})/\text{Pf}\alpha$ in terms of different U ranges are listed in Table A6. The rms scatter of the piecewise fitting correlations relative to the model results is of ~ 0.01 – 0.02 dex. The accurate metallicity calibration here depends on reliable estimates of U and E_{peak} . The former can be accurately estimated as discussed in Section 3.1, while the latter needs to be estimated iteratively together with the metallicity.

In addition, through the same feature extraction process as detailed in Section 3.1, we find that besides the relative intensities of the infrared neon and argon emission to ionized hydrogen emission, the line ratios of the infrared neon and argon emission to singly ionized iron emission can, in theory, also be used to calibrate metallicity in AGN. In particular, the line ratios involving singly ionized neon or argon (e.g., $[\text{Ar II}] 6.99 \mu\text{m}/[\text{Fe II}] 5.34 \mu\text{m}$) have an almost linear dependence on metallicity in AGN models. This result is plausibly due to the

strong dependence of iron depletion by dust on metallicity (e.g., B. O’Halloran et al. 2008). As illustrated in Figure 5 and described by Equation (10):

$$12 + \log(\text{O}/\text{H}) = c_2 \times (\log R)^2 + c_1 \times \log R + c_0. \quad (10)$$

We simply adopt a quadratic function to calibrate the metallicity with $R = [\text{Ar II}] 6.99 \mu\text{m}/[\text{Fe II}] 5.34 \mu\text{m}$ (also for $[\text{Ne II}] 12.81 \mu\text{m}/[\text{Fe II}] 5.34 \mu\text{m}$, $[\text{Ar II}] 6.99 \mu\text{m}/[\text{Fe II}] 25.99 \mu\text{m}$, and $[\text{Ne II}] 12.81 \mu\text{m}/[\text{Fe II}] 25.99 \mu\text{m}$, which are more susceptible to dust extinction corrections), and the best-fit coefficients are listed in Table A7.²⁹

The metallicity calibrated based on $[\text{Ar II}] 6.99 \mu\text{m}/[\text{Fe II}] 5.34 \mu\text{m}$ has a larger uncertainty than that calibrated based on $([\text{Ar III}] 8.99 \mu\text{m} + [\text{Ar V}] 7.90 \mu\text{m})/\text{Pf}\alpha$. This larger uncertainty is mainly due to the dependence of $[\text{Ar II}] 6.99 \mu\text{m}/[\text{Fe II}] 5.34 \mu\text{m}$ (the same for $[\text{Ne II}] 12.81 \mu\text{m}/[\text{Fe II}] 5.34 \mu\text{m}$) on gas pressure (see Figure 5(c)). Specifically, the collisional de-excitation of $[\text{Fe II}]$ is enhanced relative to the radiative de-excitation at high gas pressure (equally high gas density), given its relatively low critical electron density $\log(n_c/\text{cm}^{-3}) = 2.48$. Line ratios involving $[\text{Fe II}] 25.99 \mu\text{m}$ are less sensitive to gas pressure but are more susceptible to dust

²⁹ The calibration of metallicity using $[\text{Ar II}] 6.99 \mu\text{m}/[\text{Fe II}] 5.34 \mu\text{m}$ and $[\text{Ne II}] 12.81 \mu\text{m}/[\text{Fe II}] 5.34 \mu\text{m}$ presented here is only for $\log(P/k) \leq 8.0$ given the strong dependence of $[\text{Fe II}] 5.34 \mu\text{m}$ on gas pressure.

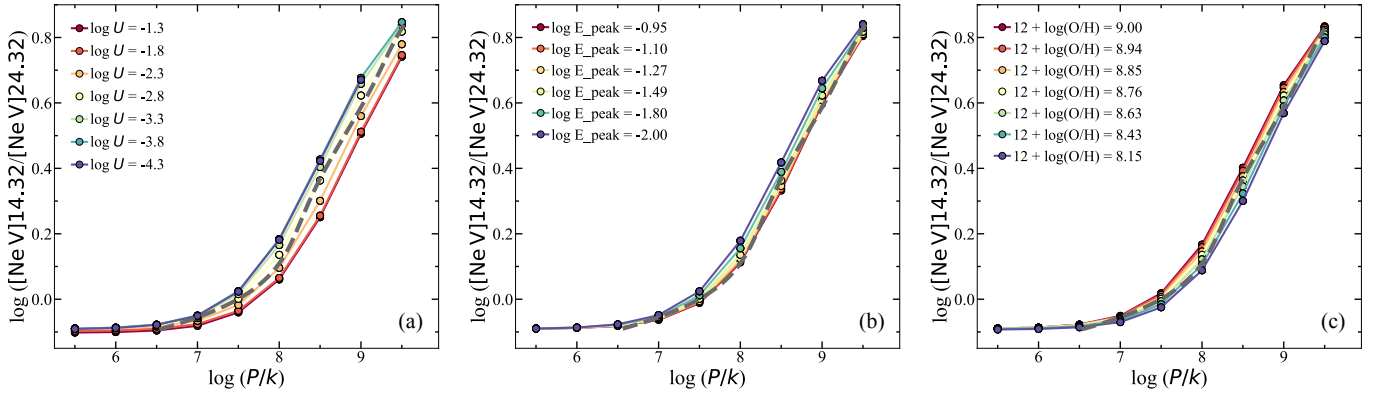


Figure 6. Dependence of $[\text{Ne V}] 14.32 \mu\text{m}/[\text{Ne V}] 24.32 \mu\text{m}$ on the gas pressure (P/k , in units of K cm^{-3}), as predicted by AGN photoionization models (colored points). Each panel displays model results under specific parameter constraints: (a) $\log E_{\text{peak}} = -1.49$ and $12 + \log(\text{O}/\text{H}) = 8.76$; (b) $\log U = -2.8$ and $12 + \log(\text{O}/\text{H}) = 8.76$; and (c) $\log U = -2.8$ and $\log E_{\text{peak}} = -1.49$, while the gray dashed line represents the best-fit correlation (Equation (10)) derived from all AGN models with $\log(P/k) \gtrsim 6.5$.

extinction corrections. Moreover, the metallicity calibrations involving iron emission lines are susceptible to dust depletion variations (e.g., C. Konstantopoulou et al. 2022, 2024; A. Hamanowicz et al. 2024). $[\text{Fe II}]$ emission is also sensitive to shock excitation that is prevalent in AGN, especially in low-luminosity AGN (see Section 4.1.2). Another caveat regarding the use of the low-excitation infrared-line ratios to calibrate metallicity, as well as other parameters, in AGN will be discussed in Section 4.1.1. Considering these caveats, we propose that $[\text{Ar II}] 6.99 \mu\text{m}/[\text{Fe II}] 5.34 \mu\text{m}$ (the same for $[\text{Ne II}] 12.81 \mu\text{m}/[\text{Fe II}] 5.34 \mu\text{m}$, $[\text{Ar II}] 6.99 \mu\text{m}/[\text{Fe II}] 25.99 \mu\text{m}$, and $[\text{Ne II}] 12.81 \mu\text{m}/[\text{Fe II}] 25.99 \mu\text{m}$) can only be used for prior estimates in relatively low-density environments, while the high-excitation-line diagnostic, i.e., $([\text{Ar III}] 8.99 \mu\text{m} + [\text{Ar V}] 7.90 \mu\text{m})/\text{P}\alpha$, should be used for more robust iterative estimates of metallicity in AGN.

3.4. Pressure Diagnostics

The ratios of emission lines of the same ion species but with different critical densities have been widely used as electron density or equivalently gas pressure diagnostics in AGN (e.g., T. Alexander et al. 1999; M. A. Dopita et al. 2002; R. P. Dudik et al. 2007; P. Zhu et al. 2024). Several such emission-line ratios are available with JWST/MRS spectral observations (i.e., $[\text{Fe VII}] 7.82 \mu\text{m}/[\text{Fe VII}] 9.53 \mu\text{m}$, $[\text{Ne V}] 14.32 \mu\text{m}/[\text{Ne V}] 24.32 \mu\text{m}$, $[\text{Ar V}] 7.90 \mu\text{m}/[\text{Ar V}] 13.10 \mu\text{m}$, $[\text{Ar III}] 8.99 \mu\text{m}/[\text{Ar III}] 21.83 \mu\text{m}$, and $[\text{Fe II}] 25.99 \mu\text{m}/[\text{Fe II}] 5.34 \mu\text{m}$). We have examined and found that $[\text{Ne V}] 14.32 \mu\text{m}/[\text{Ne V}] 24.32 \mu\text{m}$ is the best among these infrared-line pairs for diagnosing gas pressure in AGN. $[\text{Ne V}] 14.32 \mu\text{m}/[\text{Ne V}] 24.32 \mu\text{m}$ can be used to diagnose gas pressure in AGN with $\log(P/k) \gtrsim 6.5$, while the other infrared-line ratios involved here are insensitive to gas pressure until $\log(P/k) \gtrsim 7.5$ (with an n_{H} of $\sim 10^3 \text{ cm}^{-3}$). $[\text{Ne V}] 14.32 \mu\text{m}/[\text{Ne V}] 24.32 \mu\text{m}$ also has the advantage of being unaffected by starburst activity and dust depletion.

As shown in Figure 6, we include more AGN models with higher gas pressure to better depict the dependence of $[\text{Ne V}] 14.32 \mu\text{m}/[\text{Ne V}] 24.32 \mu\text{m}$ on gas pressure. We again adopt a quintic function, i.e., Equation (11):

$$\log(P/k) = c_5 \times (\log R)^5 + c_4 \times (\log R)^4 + c_3 \times (\log R)^3 + c_2 \times (\log R)^2 + c_1 \times \log R + c_0, \quad (11)$$

with $R = [\text{Ne V}] 14.32 \mu\text{m}/[\text{Ne V}] 24.32 \mu\text{m}$ to calibrate the gas pressure, and the best-fit coefficients are listed in Table A8. Note that the adopted calibration is fitted based on the data points with $\log(P/k) \gtrsim 6.5$ and the corresponding rms uncertainty is 0.19 dex.

3.5. Applications and Caveats of the Diagnostics

3.5.1. Example Applications of the Diagnostics

In the above subsections, we scrutinized the correlations between different line ratios and physical parameters and proposed optimal diagnostics for these physical parameters in a self-consistent manner. In this subsection, we apply these diagnostics to the central $1''.5 \times 1''.5$ ($\sim 200\text{--}300 \text{ pc}$ in physical scales) regions of a sample of six type 1.9–2 Seyferts as a proof of concept. The six Seyferts are included in the Galaxy Activity, Torus, and Outflow Survey (GATOS),³⁰ and were observed by MRS integral field units (IFUs) via the JWST Cycle 1 GO program (#1670; PI: T. T. Shimizu). A series of papers from the GATOS collaboration provided in-depth discussions of different aspects of one or more of the six targets, including their molecular/ionic emission lines, PAH features, ice/dust properties, and AGN feedback processes such as shocks and outflows (A. Alonso Herrero et al. 2023; R. Davies et al. 2024; F. Esposito et al. 2024; I. García-Bernete et al. 2024a, 2024b; S. García-Burillo et al. 2024; L. Hermosa Muñoz et al. 2024; L. Zhang et al. 2024b, 2024a; D. Delaney et al. 2025; D. Esparza-Arredondo et al. 2025; O. González-Martín et al. 2025).

According to the measured line ratios listed in Table 2 and the calibrations proposed in Section 3.1, the six Seyferts have $\log U$ values of ~ -2.6 to -2.4 . As a comparison, the $\log U$ values measured here are consistent with the measurements by R. Davies et al. (2020) within 0.2 dex for ESO137–G034, MCG–05–23–016, NGC 3081, and NGC 5728, and are larger by ~ 0.4 dex and ~ 0.7 dex for NGC 5506 and NGC 7172, respectively. The U values in R. Davies et al. (2020) were derived with optical $[\text{O III}] \lambda 5007/\text{H}\beta$ and $[\text{N II}] \lambda 6584/\text{H}\alpha$ line ratios measured for a slightly larger ($1''.8 \times 1''.8$) aperture from Very Large Telescope (VLT)/X-shooter IFU mode observations, and adopted the U calibration by D. Baron & H. Netzer (2019) based on theoretical calculations by

³⁰ <https://gatos.myportfolio.com>

Table 2
Nuclear Emission-line Ratios of Sample Seyferts

Target (1)	$\log \frac{[\text{Ar V}]7.90}{[\text{Ar III}]8.99}$ (2)	$\log \frac{[\text{Ar V}]13.10}{[\text{Ne III}]15.56}$ (3)	$\log \frac{[\text{Ne V I}]7.65}{[\text{Ar V}]7.90}$ (4)	$\log \frac{([\text{Ar III}]8.99 + [\text{Ar V}]7.90)}{\text{P}\alpha}$ (5)	$\log \frac{[\text{Ne V}]14.32}{[\text{Ne V}]24.32}$ (6)	$\log \frac{[\text{Ne V I}]7.65}{[\text{Fe II}]5.34}$ (7)	$\log \frac{[\text{Ar V}]7.90}{[\text{Fe II}]5.34}$ (8)
ESO137–G034	-0.70 ± 0.11	-1.45 ± 0.07	1.15 ± 0.20	1.00 ± 0.11	0.05 ± 0.08	0.76 ± 0.17	-0.39 ± 0.10
MCG–05–23–016	-0.65 ± 0.07	-1.55 ± 0.18	1.41 ± 0.04	0.69 ± 0.07	0.17 ± 0.13	1.84 ± 0.03	0.43 ± 0.05
NGC 3081	-0.75 ± 0.03	-1.44 ± 0.01	1.33 ± 0.03	1.37 ± 0.03	0.09 ± 0.01	1.79 ± 0.02	0.46 ± 0.04
NGC 5506	-0.60 ± 0.03	-1.32 ± 0.09	1.04 ± 0.04	0.74 ± 0.03	0.24 ± 0.05	0.71 ± 0.02	-0.33 ± 0.03
NGC 5728	-0.52 ± 0.14	-1.43 ± 0.06	1.22 ± 0.15	1.05 ± 0.14	0.12 ± 0.03	1.09 ± 0.06	-0.13 ± 0.14
NGC 7172	-0.54 ± 0.18	-1.50 ± 0.24	1.38 ± 0.03	0.65 ± 0.18	0.11 ± 0.19	1.02 ± 0.03	-0.36 ± 0.04

Note. Based on the measurements from the central $r = 0''.75$ (~ 100 – 150 pc) regions of the sample Seyferts by L. Zhang et al. (2024b).

CLOUDY. The different U values measured for the latter two Seyferts can be attributed to their edge-on gas disks blocking most of the optical emission lines emanating from the nuclear region, as discussed at the end of this subsection.

As discussed in Section 3.2, the $[\text{Ne VI}] 7.65 \mu\text{m}/[\text{Ar V}] 7.90 \mu\text{m}$ ratio is in principle the best E_{peak} diagnostic within JWST/MRS bands. The observed $[\text{Ne VI}] 7.65 \mu\text{m}/[\text{Ar V}] 7.90 \mu\text{m}$ line ratios indicate equivalent $\log(E_{\text{peak}}/\text{keV})$ values of ~ -1.0 to -0.5 in the central ~ 200 – 300 pc regions of the six Seyferts. These values are larger by ~ 1 dex than what would be expected from the correlation between E_{peak} and λ_{Edd} (A. D. Thomas et al. 2016) given their λ_{Edd} of ~ 0.01 – 0.06 (T. Caglar et al. 2020). On the other hand, with the $\log(E_{\text{peak}}/\text{keV})$ values of ~ -1.0 to -0.5 , the bolometric luminosities of the input AGN ionizing spectra will be over $10^{45} \text{ erg s}^{-1}$. This value exceeds the measured bolometric luminosities of $\sim 10^{43.4}$ – $10^{44.3} \text{ erg s}^{-1}$ for the six targets reported by R. I. Davies et al. (2015), indicating the need for additional heating sources beyond the AGN. A significantly higher abundance of neon relative to argon in these targets than that adopted in the modeling can also result in an overestimation of E_{peak} . However, this is not the case here because the two U values calibrated with $[\text{Ar V}] 7.90 \mu\text{m}/[\text{Ar III}] 8.99 \mu\text{m}$ and $[\text{Ar V}] 13.10 \mu\text{m}/[\text{Ne III}] 15.56 \mu\text{m}$ are consistent within 0.1 dex for all of the six targets.

A more plausible explanation for the elevated E_{peak} is the presence of an extra heating source of soft (~ 0.2 – 2 keV) X-ray to the coronal line $[\text{Ne VI}] 7.65 \mu\text{m}$ in the nuclear regions of the six Seyferts. Although the adopted AGN ionizing radiation sources in our AGN models have included the soft X-ray excess associated with the accreting black hole, emission from circumnuclear hot gas or other potential sources can further contribute to the soft X-ray radiation in AGN (see the review by B. R. McNamara & P. E. J. Nulsen 2007). Specifically, there is growing evidence that fast radiative shocks are required to explain the extension of coronal emission in AGN on scales of hundreds of parsecs, which cannot be explained by pure AGN photoionization (e.g., A. Rodríguez-Ardila et al. 2006, 2011, 2017, 2025; X. Mazzalay et al. 2010, 2013; M. Durré & J. Mould 2018; D. May et al. 2018). We examined and found that the observed $[\text{Fe VIII}] 5.45 \mu\text{m}/[\text{Mg V}] 5.61 \mu\text{m}$ ratio, a less reliable diagnostic of E_{peak} (see Section 3.2), also indicates an elevated E_{peak} , albeit with larger scatter, in the nuclear regions of all the six targets.

The derived metallicities in the central regions of the six Seyferts based on $([\text{Ar III}] 8.99 \mu\text{m} + [\text{Ar V}] 7.90 \mu\text{m})/\text{P}\alpha$ and using the above $\log(E_{\text{peak}}/\text{keV})$ values range from ~ 0.2 to $0.9 Z_{\odot}$, consistent in statistics with the metallicity distribution of type 2 Seyferts (e.g., T. Nagao et al. 2006;

O. L. Dors et al. 2019; M. Armah et al. 2023), especially within their central regions (M. Armah et al. 2024). The corresponding gas pressures $\log(P/k)$ based on $[\text{Ne V}] 14.32 \mu\text{m}/[\text{Ne V}] 24.32 \mu\text{m}$ are ~ 7.8 – 8.3 . Since the calibrations of metallicity based on $([\text{Ar III}] 8.99 \mu\text{m} + [\text{Ar V}] 7.90 \mu\text{m})/\text{P}\alpha$ has a weak dependence on E_{peak} (see Figure 4(b)), we artificially reduce the above E_{peak} values derived from $[\text{Ne VI}] 7.65 \mu\text{m}/[\text{Ar V}] 7.90 \mu\text{m}$ by 1 dex considering the potential contribution of radiative shocks to the coronal line $[\text{Ne VI}] 7.65 \mu\text{m}$, and repeat the metallicity calibration to quantify the uncertainty associated with the elevated E_{peak} . Specifically, the reduced E_{peak} leads to an increase in the metallicity of ~ 0.1 – $0.3 Z_{\odot}$ for the six targets except for NGC 3081. For the nuclear region of NGC 3081, which has the most elevated $\log(E_{\text{peak}}/\text{keV})$ value of -0.5 , the corresponding metallicity increases from $0.9 Z_{\odot}$ to $2.5 Z_{\odot}$. The relatively higher metallicity in the nuclear region of NGC 3081 is consistent with its nature as a massive, early-type barred galaxy, which tends to accumulate more stellar mass and enrich its central region due to a deeper gravitational potential.

The subsolar to solar metallicity in the central regions of the six Seyferts is itself an interesting result. A subsolar metallicity in a galaxy’s central region is generally associated with circumnuclear gas inflows, which are observed in these Seyferts (e.g., A. Schnorr-Müller et al. 2016; T. T. Shimizu et al. 2019; D. Esparza-Arredondo et al. 2025). Circumnuclear gas inflows can result in black hole growth as well as nuclear starbursts. We therefore examined the contamination effect of potential nuclear starbursts in estimating the metallicity, and found it is negligible or within an increase of $0.2 Z_{\odot}$, when their contribution to the $[\text{Ar III}] 8.99 \mu\text{m}$ and $\text{P}\alpha$ emission of the six targets is less than 30% or not exceeding 50%. Another possibility that deserves further specific study is that the mid-IR emission-line-based metallicity calibration, as well as the calibrations of other parameters discussed here, are more sensitive to the physical condition of the ISM immediately adjacent to the central ionizing source, because of the stronger penetrating power of infrared emission lines. On the contrary, optical emission lines from the inner region can be highly blocked. That is, infrared and optical diagnostics are tracking the physical conditions at different depths around ionized sources. As will be discussed in Section 4.1.1 and references therein, $[\text{Ar III}]$ and $[\text{Ar V}]$ emission lines are all emanating from H II regions (i.e., where H atoms are fully ionized) adjacent to the ionizing sources.

The hypothesis that infrared and optical diagnostics essentially trace different layers around ionizing sources can to a certain degree reconcile the larger $\log U$ estimated based on mid-IR emission lines than those estimated based on optical

emission lines for NGC 5506 and NGC 7172. These two Seyferts, especially the latter, have an edge-on gas disk that largely blocks optical emission lines from the nuclear region (S. Smajić et al. 2012; A. Alonso Herrero et al. 2023; F. Esposito et al. 2024; I. García-Bernete et al. 2024b), leaving only the portion from the periphery, and therefore decrease the log U value estimated based on the optical emission-line ratios. The correction for dust extinction of the optical emission lines applying the same extinction strength (i.e., A_V) cannot eliminate the differences in U values estimated based on optical and infrared emission-line ratios for the following reasons. First, [O III] $\lambda 5007/H\beta$, [N II] $\lambda 6584/H\alpha$, [Ar V] $7.90 \mu\text{m}/[\text{Ar III}] 8.99 \mu\text{m}$, and [Ar V] $13.10 \mu\text{m}/[\text{Ne III}] 15.56 \mu\text{m}$ are not sensitive to dust extinction corrections given the close wavelengths of these line ratios and the weak dust extinction in the mid-IR. Second, the differences in U values are more likely due to the absolute extinction of the optical emission lines in the inner region rather than partial attenuation, whereas the former effect cannot be corrected by a single extinction strength for all lines.

Furthermore, based on the optical $R(\text{N2}, \text{S2}, \text{O3})^{31}$ prescription of P. Zhu et al. (2024) and available emission-line ratios extracted from $1''8 \times 1''8$ apertures of VLT/X-shooter IFU mode observations by L. Burtscher et al. (2021), the derived metallicities for five of the six Seyferts range from ~ 1.7 to $3.5 Z_\odot$ assuming the same abundance scaling relations as adopted in this paper (i.e., D. C. Nicholls et al. 2017). Moreover, based on the $R([\text{S II}] \lambda 6717/[\text{S II}] \lambda 6731)$ prescription of P. Zhu et al. (2024) and [S II] emission-line ratios extracted from $1''8 \times 1''8$ apertures of VLT/X-shooter IFU mode observations by R. Davies et al. (2020), the derived log (P/k) values are ~ 6.9 – 7.6 for the six targets. The overall higher metallicity and correspondingly lower gas pressures derived based on optical emission lines again suggest that infrared and optical diagnostics essentially trace different layers around ionizing sources, albeit more convincing conclusions require further dedicated, especially spatially resolved, studies.

3.5.2. General Applications of the Diagnostics

We discussed above example applications of the proposed diagnostics to six Seyferts, and for more general applications in future work, we suggest following the steps summarized below. First, the ionization parameter can be derived using Equation (1) with $R = [\text{Ar V}] 7.90 \mu\text{m}/[\text{Ar III}] 8.99 \mu\text{m}$ or $[\text{Ar V}] 13.10 \mu\text{m}/[\text{Ne III}] 15.56 \mu\text{m}$ (see Section 3.1). Then, with the derived ionization parameter, the peak energy and metallicity can be iteratively derived using Equations (2) with $R = [\text{Ne VI}] 7.65 \mu\text{m}/[\text{Ar V}] 7.90 \mu\text{m}$ (see Section 3.2) and Equations (6) with $R = ([\text{Ar III}] 8.99 \mu\text{m} + [\text{Ar V}] 7.90 \mu\text{m})/\text{Pf}\alpha$ (see Section 3.3). We assume solar metallicity in the first iteration and stop the iterations when the peak energy and metallicity converge to final values. At this step, it is important to account for the contribution of radiative shocks to coronal emission lines in AGN; otherwise, these contributions could bias the diagnostics of the AGN spectral peak energy and, consequently, the inferred metallicity (see further discussion in Section 4.3). Specifically, A. Rodríguez-Ardila et al. (2025) found that radiative shocks may contribute up to 80% of the

highly ionized coronal emission lines [Fe VII] and [Fe X] in AGN. Finally, the gas pressure can be derived using Equation (11) with $R = [\text{Ne VI}] 7.65 \mu\text{m}/[\text{Ar V}] 7.90 \mu\text{m}$ (see Section 3.4), which is related to the gas density via the equation of state. Although the above steps are recommended, Equations (2) and (6) can also be used individually if the required secondary parameters (i.e., log U and $12 + \log(\text{O}/\text{H})$ or log E_{peak}) are already known. To obtain more robust statistics, we suggest perturbing the observed diagnostic emission-line fluxes with random noise at their uncertainty levels, and repeating this e.g., 100 times via Markov Chain Monte Carlo sampling. The resulting 100 sets of line ratios can then be input into Equations (1)–(11), and adopt the corresponding median and standard deviation of the 100 calculations as the final estimate and uncertainty of each physical parameter.

4. Discussion

4.1. Diagnostics in Low-luminosity Active Galactic Nuclei

As noted in Section 3.1, the AGN photoionization models produce $[\text{Ne VI}] 7.65 \mu\text{m}/[\text{Ar V}] 7.90 \mu\text{m}$ values with a bivaluation dependence on E_{peak} , which is checked to be mainly due to the nonlinear dependence of $[\text{Ne VI}] 7.65 \mu\text{m}$ emissivity on E_{peak} . Taking this into consideration, we perform independent calibrations for AGN models with $\log(E_{\text{peak}}/\text{keV}) \leq -2.25$ (empirically $\log \lambda_{\text{Edd}} \leq -3$) and therefore low luminosity (low-luminosity AGN hereafter), using the same strategies as described by Equations (1)–(11). As shown by Figures A1–A5 in the Appendix, the strategies adopted for AGN models with relatively high E_{peak} are also applicable to AGN models with relatively low E_{peak} , but with numerically different best-fit coefficients and rms scatter as listed in the Appendix.

Nevertheless, we note here that the calibrations for low-luminosity AGN in the Appendix should be used with caution, since the advection-dominated accretion flow model (see the reviews by R. Narayan & J. E. McClintock 2008; F. Yuan & R. Narayan 2014) is in principle better than OPTXAGNF in calculating the AGN ionizing spectra of these low-luminosity AGN. We keep these calibrations for the sake of completeness and in order to highlight the two factors deserving specific discussion given their potential impact on the proposed diagnostics in low-luminosity AGN. While the first factor does not significantly affect the proposed diagnostics, the second factor may have a large impact, as discussed below.

4.1.1. The Effect of Hard X-Ray Photons

The theoretical AGN photoionization models used here adopt an essentially unchanged shape (i.e., Γ) and contribution (i.e., f_{pl}) of the hard (~ 2 – 10 keV) X-ray Comptonization in AGN ionizing spectra. This is a simplified assumption, since Γ tends to decrease as the Eddington ratio of the AGN decreases, resulting in a higher fraction (f_{pl}) of hard X-ray photons in low-luminosity AGN (e.g., O. Shemmer et al. 2006; C. Done et al. 2012; C. Jin et al. 2012). Hard X-ray photons are able to penetrate deeper to further irradiate atomic/molecular gas clouds than UV photons, given the greatly reduced photoionization cross sections of H and He in the X-ray regime. This effect of X-ray photons leads to an extra excitation of heavy elements in so called X-ray dissociation regions (or X-ray-dominated regions (XDRs); P. R. Maloney et al. 1996), which

³¹ $\log R(\text{N2}, \text{S2}, \text{O3}) = 0.9738 \times \log([\text{N II}] \lambda 6584/[\text{S II}] \lambda \lambda 6717, 6731) + 0.047 \times \log([\text{N II}] \lambda 6584/H\alpha) - 0.183 \times \log([\text{O III}] \lambda 5007/H\beta)$.

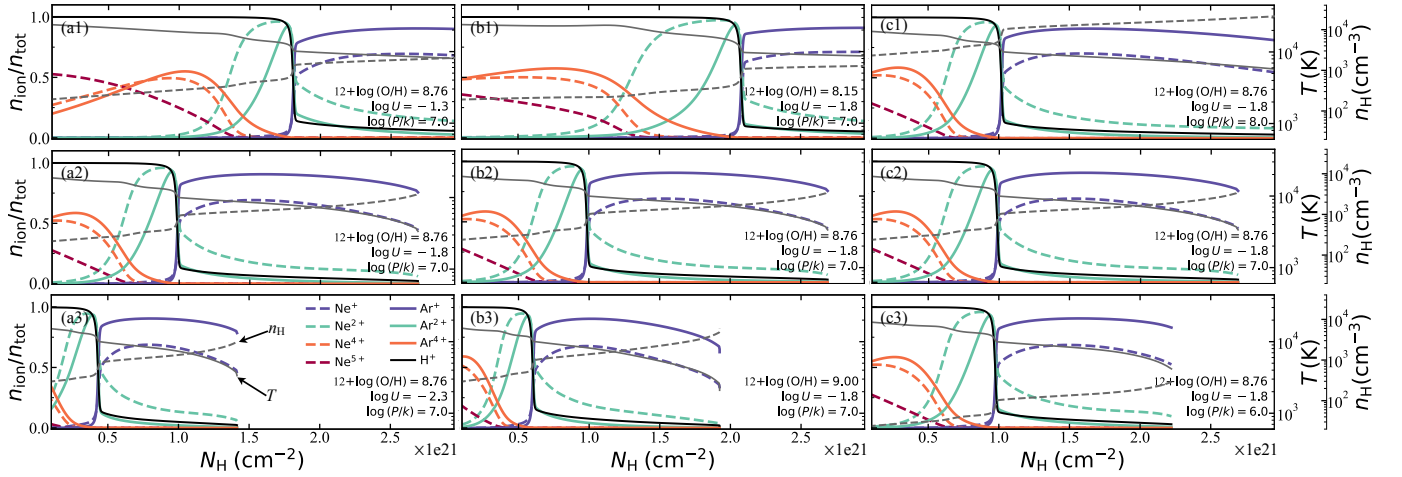


Figure 7. Examples of the ionization structures at different depths into the ionized clouds, as predicted by AGN photoionization models with the black hole mass set as $10^7 M_{\odot}$ and $\log \lambda_{\text{Edd}} = -0.5$. See the lower right of each panel for the values of other input parameters, i.e., $\log U$, $\log(P/k)$, and $12 + \log(O/H)$. The colored solid and dashed lines in each panel represent the abundances of different argon and neon ions relative to the total argon or neon abundance, respectively. As a reference, the black solid line in each panel represents the hydrogen ion abundance relative to the total hydrogen abundance. In addition, the gray solid and dashed lines in each panel, as labeled in panel (a3), represent the temperature T and column density (n_{H}) as a function of the number density (N_{H}), respectively (see the two y-axes on the right).

contribute independently to specific infrared emission lines (e.g., R. Meijerink et al. 2007; G. J. Ferland et al. 2013). The theoretical AGN photoionization models used here do not stop until the hydrogen becomes 99% neutral and therefore include the XDR contribution. In practical applications, line ratio diagnostics involving emission lines with undetermined XDR contributions have larger uncertainty than those involving only NLR emission lines (e.g., M. Pereira-Santaella et al. 2017).

Specifically, hard X-ray photons affect heavy elements (e.g., C, N, O, Ne, Na, Mg, Si, S, Ar, and Fe) mainly through the K- and L-shell photoionization, which results in multiply charged ions via the Auger effect. These highly charged ions are rapidly destroyed through charge exchange reactions with atomic and molecular hydrogen, and other species (N. P. Abel et al. 2009; M. Ádámkóvics et al. 2011). However, the contribution of XDRs in the excitation of infrared emission lines is significant for singly and doubly charged ions due to their limited charge exchange reactions with atomic and molecular hydrogen (A. E. Glassgold et al. 2007; M. Ádámkóvics et al. 2011; G. J. Ferland et al. 2013). M. Pereira-Santaella et al. (2017) found that XDR excitation can contribute, respectively, to $\sim 80\%$ and $\sim 20\%$ of the [Ne II] $12.81 \mu\text{m}$ and [Ne III] $15.56 \mu\text{m}$ emission lines in AGN models with solar metallicity, and these values decrease as metallicity increases. Relevant to this, I. García-Bernete et al. (2017) found that [Ne II] $12.81 \mu\text{m}$ and [Ne III] $15.56 \mu\text{m}$ emission show considerable correlations with X-ray continuum from 3 to 40 keV bands.

The line ratio diagnostics proposed in this study for AGN are essentially based on the emission lines of highly charged ions (i.e., [Ar III], [Ar V], [Ne V], and [Ne VI]), which are basically only radiated from H II regions with the contribution outside H II regions less than $\sim 5\%$ (see Figure 7). Therefore, the line ratio diagnostics proposed here are overall immune to the impact of XDRs, except for the line ratio diagnostics involving singly and some doubly charged ions; for example, the [Ar II] $6.99 \mu\text{m}$ /[Fe II] $5.34 \mu\text{m}$ diagnostic discussed in Section 3.3, and such diagnostics should be used with additional caution. We want to highlight again that the proposed optimal diagnostics (excluding the gas pressure

diagnostic in AGN) are all based on emission lines with $\log n_{\text{c}} \geq 4.5$ (see Table 1). Such a high critical electron density relative to the available electron density in NLRs largely eliminates the dependence of these proposed diagnostics on the gas density, and equivalently the gas pressure (see the right column of Figure 7). Moreover, the ions of these noble gases, i.e., argon and neon, are immune to the dust depletion effect and other metallicity relevant effects.

4.1.2. The Effect of Shocks

An important heating mechanism in AGN, especially in low-luminosity AGN, is shock heating (see the review by B. R. McNamara & P. E. J. Nulsen 2007), also known as kinetic mode AGN feedback and widely embraced in modern cosmological simulations (e.g., R. Weinberger et al. 2017; R. Davé et al. 2019). Since shocks are prevalent in low-luminosity AGN due to their very low radiative efficiency (e.g., L. C. Ho et al. 2003; L. C. Ho 2009), shock excitation may have a large impact on the NLR emission-line diagnostics. To study the infrared emission-line excitation in shocked regions, we use the same MAPPINGS V code to create a grid of radiative shock models as detailed by R. S. Sutherland & M. A. Dopita (2017). The corresponding radiative shock precursor, which can play an important role in gas excitation in AGN, is also included in the shock modeling.

Following R. S. Sutherland & M. A. Dopita (2017), the four varying parameter of the radiative shock models are the metallicity from $Z = 0.2, 0.4, 0.7, 1.0, 1.3, 1.7,$ and $2.0 Z_{\odot}$; the shock velocity $v_{\text{s}} = 100, 150, 200, 300, 400, 600, 800,$ and 1000 km s^{-1} ; the preshock density $n_{\text{H}} = 1, 10, 100, 1000,$ and $10,000 \text{ cm}^{-3}$; and the magnetic to ram pressure ratio $\eta_{\text{M}} = B^2 / (4\pi\rho v_{\text{s}}^2) = 0.0, 0.0001, 0.001, 0.01,$ and 0.1 , where $0.0001, 0.01,$ and 0.1 corresponding to standard, moderate, and strong magnetic fields, respectively (see Table A2 for the modeling results). In accordance with M. G. Allen et al. (2008) and A. Alarie & C. Morisset (2019), the adopted radiative shock precursors are computed separately. Specifically, they are calculated by the MAPPINGS V photoionization module using the ionizing radiation emanating from the shock as the

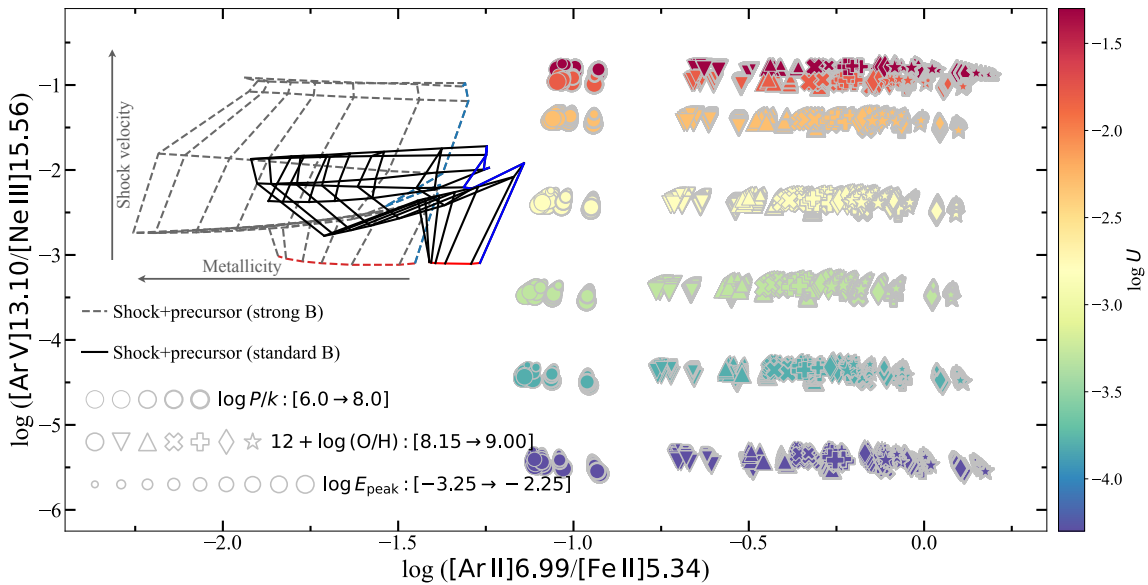


Figure 8. Diagram consisting of $[\text{Ar V}] 13.10 \mu\text{m}/[\text{Ne III}] 15.56 \mu\text{m}$ vs. $[\text{Ar II}] 6.99 \mu\text{m}/[\text{Fe II}] 5.34 \mu\text{m}$ to illustrate the contamination effects of shock excitation on emission-line ratio diagnostics in AGN. For AGN model results on the right, different colors, marker sizes, marker types, and edge widths correspond to different $\log U$, $\log E_{\text{peak}}$, $12 + \log(\text{O}/\text{H})$, and $\log(P/k)$, respectively. For the shock + precursor model results on the left, black solid and gray dashed grids correspond to model results of standard and strong magnetic fields, respectively, where the two gray arrows indicate the trend of model results as metallicity and shock velocity increase, and the red and blue lines mark the lower boundaries.

input ionizing source. The dust depletion as used in AGN models is included in the shock precursor calculations as dust can be present in radiative shock precursors albeit not in shocks (M. Pereira-Santaella et al. 2024).

As shown in Figure 8, the typical radiative shock models with $n_{\text{H}} = 100 \text{ cm}^{-3}$, $Z = 0.2-2 Z_{\odot}$, and $v_s = 100-1000 \text{ km s}^{-1}$ for standard and especially strong magnetic fields produce a range of $[\text{Ar V}] 13.10 \mu\text{m}/[\text{Ne III}] 15.56 \mu\text{m}$ values that are within the range of those produced by the AGN models. Such overlapping exists in not only U diagnostics like $[\text{Ar V}] 13.10 \mu\text{m}/[\text{Ne III}] 15.56 \mu\text{m}$ but also diagnostics of other physical parameters studied here as further discussed in Section 4.3. This conclusion does not change with different preshock densities not shown in Figure 8 and holds for the high-luminosity AGN discussed in Section 3. In other words, shocked regions can produce diagnostic emission-line ratios the same as some AGN-excited regions. Therefore, it is important to identify and exclude the contribution of shock-dominated regions when diagnosing the physical parameters of NLRs in AGN. The identification of shocked regions in AGN has been studied over decades (e.g., M. A. Dopita & R. S. Sutherland 1995; B. A. Groves et al. 2004; M. G. Allen et al. 2008; A. Alarie & C. Morisset 2019; L. J. Kewley et al. 2019; A. Feltre et al. 2023), but still deserves further specific studies under the view of JWST. Line ratios involving $[\text{Fe II}]$ emission lines as illustrated in Figure 8 are useful here because enhanced $[\text{Fe II}]$ emission in AGN is always associated with shocked regions (e.g., D. A. Forbes & M. J. Ward 1993; H. Mouri et al. 2000; T. Storchi-Bergmann et al. 2009; B.-C. Koo et al. 2016; A. Rodríguez-Ardila et al. 2017; M. Durré & J. Mould 2018). Before scrutinizing them in further specific studies, we briefly discuss the diagrams that distinguish shocked regions in AGN, and candidate strategies for quantifying the contribution of radiative shocks to gas heating in AGN later in Section 4.3.

4.2. Diagnostics in Star-forming Regions

The coevolution of galaxies and AGN has become an widely accepted notion in contemporary cosmology (see the reviews by J. Kormendy & L. C. Ho 2013; T. M. Heckman & P. N. Best 2014), and circumnuclear starbursts are prevalent in AGN (e.g., R. Cid Fernandes et al. 2001; Y. Watabe et al. 2008; M. Imanishi et al. 2011; P. Esquej et al. 2014; S. García-Burillo et al. 2014; I. García-Bernete et al. 2022; L. Zhang & L. C. Ho 2023). Similar to shock-dominated regions, star formation-dominated regions in AGN need to be distinguished and discussed regarding the diagnostics of the physical conditions specifically as well. Therefore, in this subsection we discuss the theoretical infrared-line ratio diagnostics in SF regions. The MAPPINGS V code is again used to calculate the theoretical models of SF regions using the same settings, i.e., metallicity, dust depletion, geometry, ionization parameter, gas pressure, stop criterion, etc., as the AGN models, but with different ionizing radiation fields (see Table A3 for the modeling results).

The ionizing radiation fields for the SF models are adopted from A. D. Thomas et al. (2018) derived using the SLUG2 (M. R. Krumholz et al. 2015) stellar population synthesis code with the settings summarized as follows. The ionizing radiation fields are calculated for “galaxy” (continuous star formation) mode with the default Starburst99 spectral synthesis and Padova stellar tracks with thermally pulsing AGB stars, given an age of 10 million years and a star formation rate of $0.001 M_{\odot} \text{ yr}^{-1}$. The ionizing spectra were first calculated under five available metallicities $Z = 0.0004, 0.004, 0.008, 0.02, \text{ and } 0.05$, then interpolated for the ionizing spectra of the oxygen abundances as used in the AGN models. Unlike for the AGN models, the input ionizing spectra of the SF models are determined by the metallicity. As shown in Figure 9, the low-metallicity SF models have harder ionizing spectra, but still

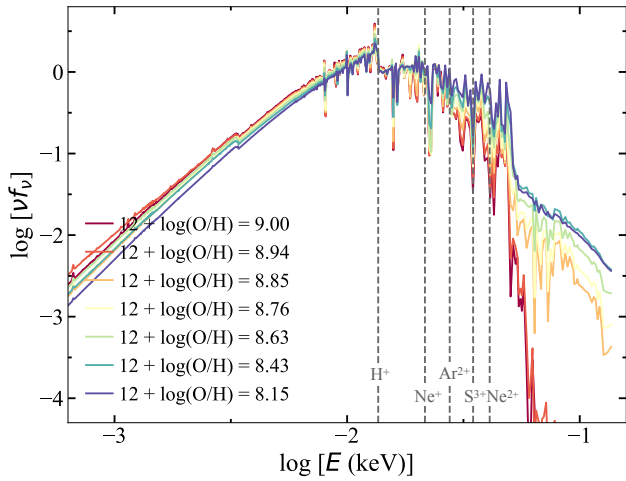


Figure 9. The ionizing spectra calculated by A. D. Thomas et al. (2018) for the SF photoionization models, where the vertical lines indicate the required ionization energy of marked ions. All ionizing spectra are normalized by the flux at the IP of hydrogen atom (i.e., 13.6 eV).

lacking high-energy photons for the excitation of high-IP lines such as [Ar V] and [Ne V].³²

We repeat the same feature extraction process as for the AGN models for the line ratios predicted by the SF models. As opposed to the AGN models (see Section 3.1), we find that the optimal line ratios for U diagnostics for the SF models are those involving [S IV] 10.51 μm , e.g., the [S IV] 10.51 μm /[Ne III] 15.56 μm line ratio as shown in Figure 10(a). This result is consistent with the previous finding by M. Pereira-Santaella et al. (2017). We adopt a cubic function, i.e., Equation (12):

$$\log U = c_3 \times (\log R)^3 + c_2 \times (\log R)^2 + c_1 \times \log R + c_0, \quad (12)$$

to calibrate U in SF regions, and the best-fit coefficients for $R = [\text{S IV}] 10.51 \mu\text{m}/[\text{Ne III}] 15.56 \mu\text{m}$ are listed in the Appendix. Quantitatively, this calibration has an rms scatter of 0.17 dex.

Contrary to the AGN models, the optimal metallicity diagnostics in the SF models are the line ratios of low-excitation neon and argon lines relative to hydrogen emission. These low-excitation lines in the SF models also have a strong dependence on the ionization parameter as those high-excitation lines in the AGN models. We therefore adopt the strategy as described by Equations (13)–(15) to calibrate the metallicity in SF regions:

$$12 + \log(\text{O}/\text{H}) = a \times (\log R - b)^2 + c, \quad (13)$$

where

$$a = a_{U,2} \times (\log U)^2 + a_{U,1} \times \log U + a_0, \quad (14)$$

$$b = b_{U,2} \times (\log U)^2 + b_{U,1} \times \log U + b_0, \quad (15)$$

$$c = c_{U,2} \times (\log U)^2 + c_{U,1} \times \log U + c_0. \quad (16)$$

We propose $R = [\text{Ne II}] 12.81 \mu\text{m}/\text{P}\alpha$, as shown by Figure 10(b), for the metallicity calibration since the [Ar II] 6.99 μm emission line is weaker than the [Ne II] 12.81 μm emission line by ~ 1 – 2 orders of magnitude in the SF models.

³² [Ar V] emission is strong enough only in SF models of hard and intensive radiation fields with low metallicities and high ionization parameters.

The best-fit coefficients for $R = [\text{Ne II}] 12.81/\text{P}\alpha$, as well as [Ar II] 6.99 $\mu\text{m}/\text{P}\alpha$ with comparable rms scatter of ~ 0.02 dex, are listed in the Appendix.

The ionizing spectra of the SF models do not have a meaningful definition of E_{peak} as that of the AGN models. However, since the hardness of the SF ionizing radiation field is determined by metallicity, we can still qualitatively study some proposed radiation field hardness diagnostics for SF regions in the literature with the SF models calculated here. For example, [Ne III] 15.56 $\mu\text{m}/[\text{Ne II}] 12.81 \mu\text{m}$, [Ar III] 8.99 $\mu\text{m}/[\text{Ar II}] 6.99 \mu\text{m}$, and [S IV] 10.51 $\mu\text{m}/[\text{S III}] 18.71 \mu\text{m}$ have long been proposed to be radiation field hardness diagnostics in SF regions (e.g., M. D. Thornley et al. 2000; N. M. Förster Schreiber et al. 2001; U. Giveon et al. 2002; A. Verma et al. 2003; L. Snijders et al. 2007), we therefore check the correlations between the predicted values of these line ratios and the metallicity of the SF models. We find that for a given U , [Ne III] 15.56 $\mu\text{m}/[\text{Ne II}] 12.81 \mu\text{m}$ and [Ar III] 8.99 $\mu\text{m}/[\text{Ar II}] 6.99 \mu\text{m}$ show tight monotonic correlations with metallicity and hence the radiation field hardness of the SF models, while [S IV] 10.51 $\mu\text{m}/[\text{S III}] 18.71 \mu\text{m}$ also shows a secondary dependence on gas pressure (see Figure A6 in the Appendix). All these line ratios have a strong dependence on U , with the predicted [Ne III] 15.56 $\mu\text{m}/[\text{Ne II}] 12.81 \mu\text{m}$ and [Ar III] 8.99 $\mu\text{m}/[\text{Ar II}] 6.99 \mu\text{m}$ values are enhanced by 2 orders of magnitude, and are even larger for [S IV] 10.51 $\mu\text{m}/[\text{S III}] 18.71 \mu\text{m}$, when $\log U$ changes from -4.3 to -1.3 (see Figure A6).

Finally, two line ratio candidates for diagnosing the gas pressure in SF regions within JWST/MRS bands are [Ar III] 8.99 $\mu\text{m}/[\text{Ar II}] 6.99 \mu\text{m}$ and [Fe II] 25.99 $\mu\text{m}/[\text{Fe II}] 5.34 \mu\text{m}$, since the SF ionizing spectra do not have enough high-energy photons to excite the high-IP lines (i.e., [Fe VII], [Ne V], and [Ar V]). However, the [Ar III] 8.99 $\mu\text{m}/[\text{Ar II}] 6.99 \mu\text{m}$ ratio and the [Fe II] 25.99 $\mu\text{m}/[\text{Fe II}] 5.34 \mu\text{m}$ ratio are insensitive to gas pressure until $\log(P/k) \gtrsim 7.5$, which is beyond the gas pressure range of typical H II regions in observations (e.g., D. Pathak et al. 2025). We therefore do not provide the infrared-line-ratio-based gas pressure calibration for SF regions.

4.3. Diagrams to Distinguish Excitation Sources

From the seminal work by J. A. Baldwin et al. (1981) and the extended studies (e.g., W. C. Keel 1983; S. Veilleux & D. E. Osterbrock 1987), two-dimensional diagrams based on optical emission-line ratios are widely used to classify galaxies governed by different excitation sources, i.e., AGN, shocks, and SF activities (e.g., L. J. Kewley et al. 2001, 2006; G. Kauffmann et al. 2003). Emission-line-ratio diagrams can be used to distinguish different types of galaxies because different excitation mechanisms operating on the ISM gas result in different line ratios in observation, which can be used to infer the hidden physical properties of galactic environments (see the review by L. J. Kewley et al. 2019).

Recently, A. Feltre et al. (2023) advanced the application of such emission-line-ratio diagrams to the mid-IR band based on photoionization models and joint optical and mid-IR spectral observations of 42 Seyfert galaxies. They specifically focused on [Ne II] 12.81 μm , [Ne III] 15.56 μm , [Ne V] 14.32 μm , [S III] 18.71 μm , [S IV] 10.51 μm , and [O IV] 25.89 μm measured from Spitzer/IRS spectra and strong optical emission lines (i.e., H α , H β , [O I] $\lambda 6300$, [O III] $\lambda 5007$,

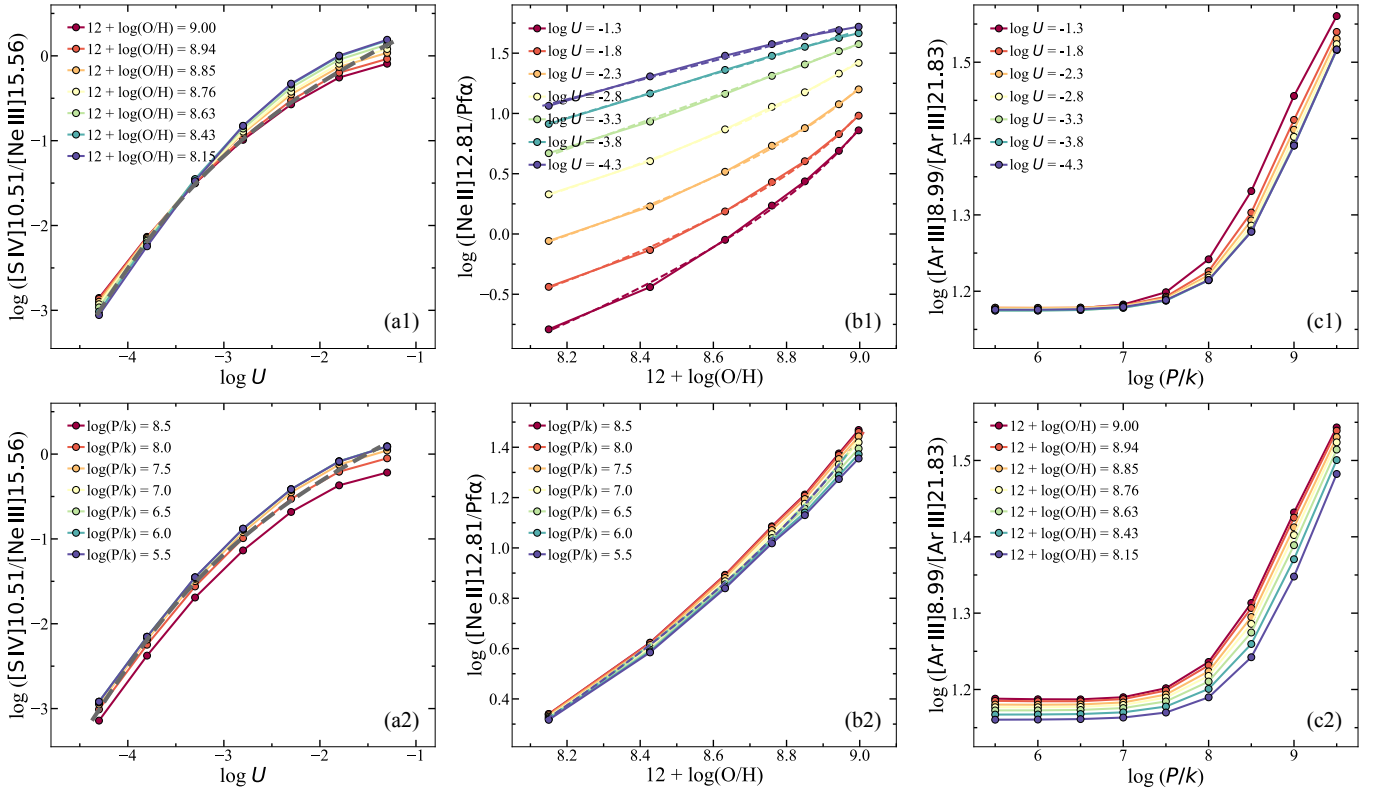


Figure 10. Dependence of (a1 and a2) $[S\text{ IV}] 10.51 \mu\text{m}/[\text{Ne III}] 15.56 \mu\text{m}$ on the ionization parameter (U); (b1 and b2) $[\text{Ne II}] 12.81 \mu\text{m}/P_f\alpha$ on the metallicity ($12 + \log(\text{O}/\text{H})$); and (c1 and c2) $[\text{Ar III}] 8.99 \mu\text{m}/[\text{Ar III}] 21.83 \mu\text{m}$ on the gas pressure (P/k), as predicted by SF photoionization models (colored points). Each panel displays model results under specific parameter constraints: (a1 and b1) $\log(P/k) = 7.0$; (c1 and a2) $12 + \log(\text{O}/\text{H}) = 8.76$; and (b2 and c2) $\log U = -2.8$. The gray dashed lines in panels (a1) and (a2) represent the best-fit correlation (Equation (12)) derived from all SF models discussed in this section, while the colored dashed lines in panels (b1) and (b2) represent the best-fit correlations (Equation (13)–(16)) derived from all SF models with the given $\log U$.

$[\text{N II}] \lambda 6584$, and $[\text{S II}] \lambda \lambda 6716, 6731$ obtained with the Southern Africa Large Telescope. They found that although the mid-IR line ratios involving $[\text{Ne V}] 14.32 \mu\text{m}$, $[\text{O IV}] 25.89 \mu\text{m}$, and $[\text{S IV}] 10.51 \mu\text{m}$ are good tracers of the AGN activity versus star formation as found in other work (e.g., L. Spinoglio & M. A. Malkan 1992; R. Genzel et al. 1998; D. A. Dale et al. 2006; L. Armus et al. 2007; C. T. Richardson et al. 2022, 2025; L. M. Feuillet et al. 2025), such line ratios also show a dependence on the AGN contribution to the mid-IR continuum. In addition, they found that star formation or radiative shocks, especially the latter, can contribute to $[\text{Ne V}] 14.32 \mu\text{m}$, $[\text{O IV}] 25.89 \mu\text{m}$, and $[\text{S IV}] 10.51 \mu\text{m}$ as well. A. Feltre et al. (2023) therefore suggested that diagrams involving only $[\text{Ne V}] 14.32 \mu\text{m}$, $[\text{S IV}] 10.51 \mu\text{m}$, or $[\text{O IV}] 25.89 \mu\text{m}$ are not sufficient to simultaneously reveal the relative roles of star formation, AGN, and shocks. This point is further demonstrated by the significant overlap in the distributions of SF, AGN, and shock models, especially the latter two, in Figure A7 in the Appendix, based on the photoionization models discussed in the above sections.

As discussed in Section 3, the mid-IR emission lines of highly ionized argon (i.e., $[\text{Ar V}]$) and neon (i.e., $[\text{Ne VI}]$) observable by JWST/MRS are effective as diagnostics of the ionization parameter and AGN spectral peak energy. In addition, as illustrated in Section 4.1.2, $[\text{Fe II}]$ emission lines are significantly enhanced in shocked regions. We therefore expect that a diagram consisting of these emission lines would be able to pick out the AGN ionized regions well. Figure 11 presents two of such diagrams consisting of (a) $[\text{Ne VI}] 7.65 \mu\text{m}/[\text{Ar V}] 7.90 \mu\text{m}$ versus $[\text{Ar V}] 7.90 \mu\text{m}/[\text{Ar III}]$

$8.99 \mu\text{m}$ and (b) $[\text{Ne VI}] 7.65 \mu\text{m}/[\text{Fe II}] 5.34 \mu\text{m}$ versus $[\text{Ar V}] 7.90 \mu\text{m}/[\text{Fe II}] 5.34 \mu\text{m}$. The colored contours in Figure 11 (as well as those in Figure A7) represent the line ratio distributions predicted by the photoionization models discussed in the above sections. The discrete distribution peaks are mainly due to the sampling effect of model grids, not necessarily reflect actual distribution peaks in observations. Compared with the diagrams in Figure A7 involving $[\text{Ne V}] 14.32 \mu\text{m}$, $[\text{O IV}] 25.89 \mu\text{m}$, and $[\text{S IV}] 10.51 \mu\text{m}$, the overall distributions of the radiative shock and AGN model predictions in Figure 11 show that it is more feasible to use diagrams involving infrared $[\text{Ne VI}]$ and $[\text{Ar V}]$ emission lines to distinguish galactic regions dominated by different excitation sources. Figure 11 does not include SF models but can still be used to indirectly distinguish SF regions because SF regions can barely produce $[\text{Ne VI}] 7.65 \mu\text{m}$ emission line due to its very high IP (126.2 eV).³³

Although better than the diagrams in Figure A7, the diagrams in Figure 11 still show overlapping areas between the radiative shock and AGN model results. This result further demonstrates that shocked regions can produce diagnostic emission-line ratios the same as some AGN-excited regions. Therefore, in order to better distinguish the dominant excitation sources in different galaxies, the two diagrams in Figure 11 should be used synergistically. Specifically, Figure 11(a) can be used to distinguish between AGN with different E_{peak} given the overall lower $[\text{Ne VI}] 7.65 \mu\text{m}/[\text{Ar V}]$

³³ For all SF models involved in this work, their $[\text{Ne VI}] 7.65 \mu\text{m}$ emission intensities are essentially less than one-millionth of the $\text{H}\beta$ emission intensity.

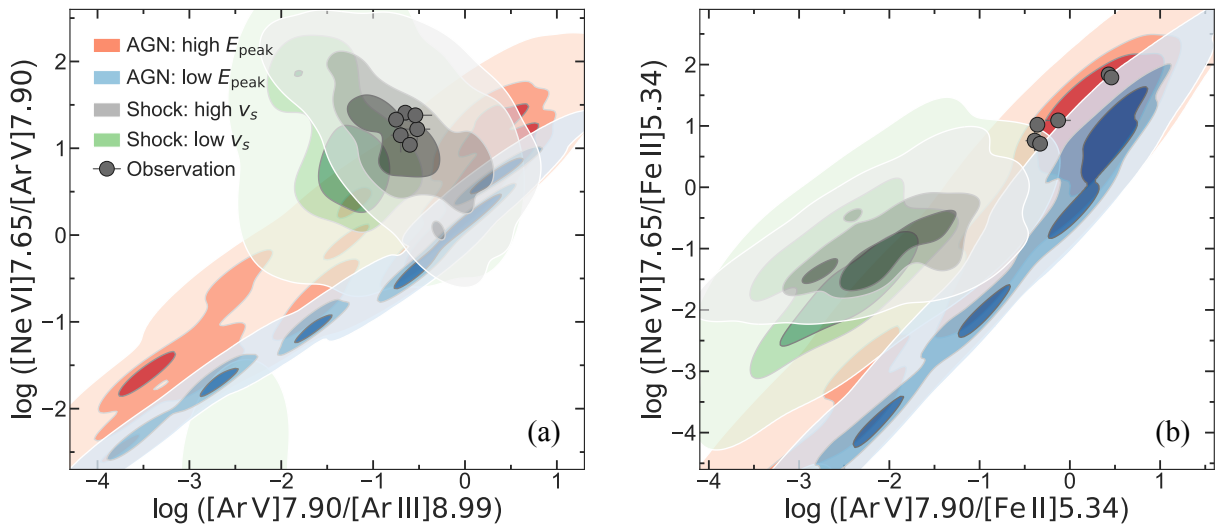


Figure 11. Diagrams consisting of (a) $[\text{Ne VI}] 7.65 \mu\text{m}/[\text{Ar V}] 7.90 \mu\text{m}$ vs. $[\text{Ar V}] 7.90 \mu\text{m}/[\text{Ar III}] 8.99 \mu\text{m}$ and (b) $[\text{Ne VI}] 7.65 \mu\text{m}/[\text{Fe II}] 5.34 \mu\text{m}$ vs. $[\text{Ar V}] 7.90 \mu\text{m}/[\text{Fe II}] 5.34 \mu\text{m}$ to distinguish between photoionization models excited by AGN and radiative shocks (i.e., including the shock precursors). Specifically, the red, blue, gray, and green contours (from dark to light covering 0%–30%, 30%–70%, and 70%–100% of the corresponding models involved in this work) represent AGN models with $-2.0 \leq \log E_{\text{peak}} \leq -0.95$ (high E_{peak}) and $-3.25 \leq \log E_{\text{peak}} \leq -2.25$ (low E_{peak}), and radiative shock models with $v_s \geq 500 \text{ km s}^{-1}$ (high v_s) and $v_s \leq 500 \text{ km s}^{-1}$ (low v_s), respectively. The six gray points represent the measurements in Table 2 of the six Seyferts discussed in Section 3.5.

$7.90 \mu\text{m}$ ratios in AGN with low E_{peak} . High- E_{peak} and low- E_{peak} AGN correspond to high and low accretion rate AGN, respectively, and can be empirically regraded as high-luminosity AGN (e.g., Seyferts) and low-luminosity AGN (e.g., LINERs). Figure 11(a) also shows that radiative shock models with $v_s \geq 500 \text{ km s}^{-1}$ have overall higher $[\text{Ne VI}] 7.65 \mu\text{m}/[\text{Ar V}] 7.90 \mu\text{m}$ ratios as well as $[\text{Ar V}] 7.90 \mu\text{m}/[\text{Ar III}] 8.99 \mu\text{m}$ ratios than radiative shock models with $v_s \leq 500 \text{ km s}^{-1}$, indicating harder radiation fields and higher ionization parameters in radiative shocks with higher velocities. This trend is even more pronounced within radiative shock precursors. Specifically, pure shock precursors (not shown here) associated with shocks of $v_s \leq 500 \text{ km s}^{-1}$ consistently lie just below the model predictions for low- E_{peak} AGN, while those with $v_s \geq 500 \text{ km s}^{-1}$ intersect the upper end of the model predictions for high- E_{peak} AGN. Contrary to Figure 11(a), Figure 11(b) does not show a clear difference in the distributions of AGN with high E_{peak} and low E_{peak} , as well as radiative shocks with high v_s and low v_s , whereas it better distinguishes radiative shocks from AGN given their overall different distributions. Combining the two diagrams in Figure 11, we find that the nuclear regions of the six targets discussed in Section 3.5 are governed by high- E_{peak} AGN, which is consistent with their nature as Seyferts.

Nevertheless, we cannot entirely rule out a scenario involving a composite contribution from both AGN and fast radiative shocks. Diagnostic diagrams involving kinematic information of the emission lines can shed more light on the existence of shocked regions (J. J. D’Agostino et al. 2019; P. Zhu et al. 2025). However, quantifying the contribution of shocked regions remains challenging, and they can contribute up to 80% of the coronal emission in AGN (A. Rodríguez-Ardila et al. 2025). This is particularly true for shocks dominated by radiation from their radiative precursors, which closely mimic the ionizing radiation fields of AGN. The approaches of constructing starburst–AGN mixing sequences—either by anchoring empirical points (e.g., L. J. Kewley et al. 2001; V. Wild et al. 2010) or by fitting multiple line ratios with model results (e.g.,

R. L. Davies et al. 2016; A. D. Thomas et al. 2018; A. Marconi et al. 2024)—are worth exploring to develop similar shock–AGN mixing sequences to help quantify the contribution of shocked regions to gas excitation in AGN. However, due to the fundamental differences in the underlying physics of shock and AGN models, constructing shock–AGN mixing sequences is inherently more complex than building starburst–AGN mixing sequences, and thus requires dedicated investigation beyond the scope of this study.

5. Summary and Conclusions

With excellent spectral and angular resolutions and, especially, sensitivity, JWST allows us to observe a variety of infrared emission lines that were previously inaccessible or barely accessible (e.g., $[\text{Ar V}] 7.90 \mu\text{m}$ and $[\text{Ne VI}] 7.65 \mu\text{m}$). Covering a wide range of critical densities and IPs (see Table 1), these infrared emission lines provide us with an unprecedented opportunity to better diagnose the physical conditions in AGN, as well as in shocks and SF regions. Based on MAPPINGS V theoretical photoionization modeling, we systematically explore the feasibility of different infrared-line combinations within the JWST/MRS $\sim 5\text{--}28 \mu\text{m}$ spectral range in diagnosing the ionization parameter (U), the peak energy of AGN ionizing spectrum (E_{peak}), metallicity ($12 + \log(\text{O}/\text{H})$), and gas pressure (P/k) in NLRs of AGN, as well as in SF regions. To find out the optimal prescriptions for the above diagnostics, we adopt a feature extraction method based on the Pearson correlation coefficient combining some practical criteria.

The main results about the infrared diagnostics can be summarized as follows.

1. Overall, the line ratios involving $[\text{Ar V}]$ (e.g., $[\text{Ar V}] 7.90 \mu\text{m}/[\text{Ar III}] 8.99 \mu\text{m}$ and $[\text{Ar V}] 13.10 \mu\text{m}/[\text{Ne III}] 15.56 \mu\text{m}$ are recommended) are the best U diagnostics for NLRs in AGN, followed by line ratios involving $[\text{Ne V}]$, and finally line ratios involving $[\text{O IV}]$ with larger scatter (see Section 3.1). In the meanwhile, the best U

- diagnostics in SF regions are line ratios involving [S IV] (e.g., [S IV] 10.51 μm /[Ne III] 15.56 μm is recommended, see Section 4.2).
2. High-IP lines (e.g., [Ne VI] 7.65 μm) are recommended to diagnose E_{peak} (essentially the radiation field hardness) in AGN, since they have, among the infrared emission lines covered by JWST/MRS spectra, the strongest dependence on E_{peak} besides the primary dependence on U . In particular, the line ratio composed of emission lines from two noble gases, i.e., [Ne VI] 7.65 μm /[Ar V] 7.90 μm , is considered to be an effective diagnostic of the AGN radiation field hardness (see Section 3.2).
 3. The intensities of highly ionized argon emission (i.e., [Ar III] 8.99 μm + [Ar V] 7.90 μm) and singly ionized neon emission ([Ne II] 12.81 μm) after normalization by hydrogen emission (i.e., Pf α) are proposed to diagnose metallicity in NLRs of AGN and in SF regions, respectively, despite them also having a primary dependence on U . The line ratios involving singly ionized neon/argon and iron (i.e., [Ar II] 6.99 μm /[Fe II] 5.34 μm and [Ne II] 12.81 μm /[Fe II] 5.34 μm) could be complementary metallicity diagnostics in AGN, but subject to dust depletion, as well as X-ray and shock excitation (see Sections 3.3 and 4.2).
 4. The ratios of infrared emission lines of the same ion species but different critical densities are explored to diagnose gas pressure in AGN and SF regions. While [Ne V] 14.32 μm /[Ne V] 24.32 μm is a good choice in diagnosing gas pressure in AGN, there is no such line ratio that can be used in SF regions (see Section 3.4). The two candidates of gas pressure diagnostic within JWST/MRS bands for SF regions, i.e., [Ar III] 8.99 μm /[Ar III] 21.83 μm and [Fe II] 25.99 μm /[Fe II] 5.34 μm , are insensitive to gas pressure until $\log(P/k) \gtrsim 7.5$, which is beyond the gas pressure range of typical H II regions in observations (see Section 4.2).

The proposed diagnostics are applicable to both high- and low-luminosity AGN and are applied to galaxies from the GATOS program. Specifically, the proposed diagnostics indicate $\log U$ values of ~ -2.6 to 2.4, $\log E_{\text{peak}}$ values of ~ -1.0 to -0.5 , metallicities of ~ 0.2 – $0.9 Z_{\odot}$, and $\log(P/k)$ values of ~ 7.8 – 8.3 in the central ~ 200 – 300 pc regions of six Seyferts (see Section 3.5). The derived $\log U$ values are overall consistent with previous measurements based on optical [O III]/H β and [N II]/H α line ratios. The derived metallicities are statistically consistent with the subsolar metallicities measured for large samples of type 2 AGN. However, the derived E_{peak} values are larger by ~ 1 dex than what would be expected from the correlation between E_{peak} and λ_{Edd} . The elevated E_{peak} is plausibly due to extra heating from the circumnuclear hot gas associated with fast radiative shocks.

Additional attention is required especially when applying these emission-line-ratio diagnostics to low-luminosity AGN (see Section 4.1), where the diagnostics could be affected by hard X-rays and potential shocks. Although the line ratio diagnostics proposed in this study for AGN are essentially based on emission lines of highly charged ions in NLRs (i.e., [Ar V], [Ne V], and Ne VI) and thus largely avoid the impact of XRDs (see Section 4.1.1), it is still crucial to identify and exclude shock-dominated regions when diagnosing the physical conditions of NLRs in AGN (see Section 4.1.2). Last but not least, further studies based on the results here are deserved to help develop new diagrams (e.g.,

[Ne VI] 7.65 μm /[Ar V] 7.90 μm versus [Ar V] 7.90 μm /[Ar III] 8.99 μm and [Ne VI] 7.65 μm /[Fe II] 5.34 μm versus [Ar V] 7.90 μm /[Fe II] 5.34 μm) for distinguishing galactic regions governed by different excitation sources, i.e., AGN, shocks, and SF activities (see Section 4.3).

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Appendix

Tables for the Modeling Results, Figures for Low-luminosity Active Galactic Nuclei, and Tables for the Coefficients of the Best-fit Correlations

Tables A1, A2, and A3 provide the model results that assume a homogeneous distribution of ionized gas for the AGN, radiative shocks, and SF regions, respectively. Figures A1–A5 are the same as Figures 2–6 in the main text but for low-luminosity AGN. Figure A6 is related to the discussion in Section 4.2 on the radiation field hardness diagnostics in SF regions. Figure A7 is related to the discussion in Section 4.3 on the mid-IR line ratio diagrams involving [Ne V] 14.32 μm , [S IV] 10.51 μm , and [O IV] 25.89 μm . Tables A4–A10 summarize the coefficients in all best-fit correlations proposed in the main text (a more user-friendly compilation of all these coefficients is available online via Zenodo at doi:10.5281/zenodo.16781788 and GitHub).³⁴

³⁴ https://github.com/LuluZhang-Astro/Data/blob/main/Coefficients_Functions.py

Table A1
The Modeling Results for the Active Galactic Nuclei

M_{BH} (1)	λ_{Edd} (2)	E_{peak} (3)	U (4)	Abundance (5)	P/k (6)	Fe II	Fe VIII	Mg VII	Mg V	Ar II	Na III	Pf α	Ne VI	Fe VII	Ar V	Ar III	Fe VII	S IV	H α	Ne II	Ar V	Ne V	Ne III	S III	Ar III	Ne V	O IV	Fe II
						5.34 μm (7)	5.45 μm (8)	5.50 μm (9)	5.61 μm (10)	6.99 μm (11)	7.32 μm (12)		7.65 μm (14)	7.82 μm (15)	7.90 μm (16)	8.99 μm (17)	9.53 μm (18)	10.51 μm (19)		12.81 μm (21)	13.10 μm (22)	14.32 μm (23)	15.56 μm (24)	18.71 μm (25)	21.83 μm (26)	24.32 μm (27)	25.89 μm (28)	25.99 μm (29)
6.0	-2.5	-1.997	-3.8	8.632	6.0	1.90e-01	nan	nan	4.42e-07	4.86e-02	5.06e-03	2.52e-02	nan	nan	2.58e-05	1.59e-01	nan	1.26e-02	9.63e-03	5.99e-01	4.45e-05	1.89e-05	1.33e+00	6.25e-01	1.09e-02	2.31e-05	4.49e-03	6.75e-02
6.0	-5.0	-2.622	-3.3	8.76	5.5	9.72e-02	nan	nan	2.40e-05	3.40e-02	5.30e-03	2.61e-02	9.62e-06	3.25e-06	4.62e-04	2.26e-01	1.20e-05	1.18e-02	1.00e-02	4.51e-01	8.12e-04	1.17e-03	1.70e+00	9.41e-01	1.53e-02	1.44e-03	1.44e-03	3.44e-02
6.0	-1.0	-1.2685	-3.8	8.76	5.5	3.86e-01	nan	nan	2.24e-06	1.62e-01	1.20e-02	2.46e-02	1.97e-06	4.54e-07	6.93e-05	2.07e-01	1.65e-06	2.53e-02	9.40e-03	1.34e+00	1.19e-04	1.11e-04	3.02e+00	1.81e-02	1.42e-02	1.37e-04	6.44e-03	1.37e-01
8.5	-2.5	-2.622	-1.8	8.632	7.0	4.98e-02	1.36e-03	9.95e-04	4.63e-02	1.88e-02	3.96e-03	2.33e-02	1.49e-01	4.85e-03	9.35e-02	7.96e-02	1.70e-02	1.74e+00	8.82e-03	1.80e-01	1.50e-01	7.82e-01	1.26e+00	5.59e-01	5.43e-03	9.12e-01	3.34e+00	1.89e-02
6.0	0.0	-0.94915	-2.3	8.85	7.5	2.43e-01	1.24e-02	1.42e-02	4.34e-02	1.63e-01	8.46e-03	1.99e-02	1.44e+00	1.51e-02	1.13e-01	1.98e-01	5.21e-02	1.15e+00	7.49e-03	1.37e+00	1.73e-01	2.02e+00	2.34e+00	2.21e-02	1.35e-02	2.17e-02	4.74e+00	9.87e-02
8.0	-3.5	-2.747	-1.3	8.76	8.0	7.56e-02	5.74e-03	8.00e-03	5.83e-02	6.17e-02	5.17e-03	2.24e-02	8.88e-01	8.92e-03	1.75e-01	8.32e-02	3.03e-02	1.70e+00	8.44e-03	5.65e-01	2.25e-01	1.69e+00	1.55e+00	6.64e-01	5.05e-02	1.35e-02	2.32e+00	4.03e-02
8.5	-1.0	-2.247	-2.3	8.943	7.0	3.75e-02	1.24e-04	1.03e-05	6.73e-03	2.81e-02	5.63e-03	2.60e-02	1.19e-02	1.01e-03	5.38e-02	2.45e-01	3.67e-03	2.07e+00	9.94e-03	3.21e-01	9.05e-02	3.02e-01	2.44e+00	1.47e-01	1.64e-02	3.32e-01	2.80e+00	1.50e-02
6.0	-4.5	-2.497	-2.3	8.15	6.0	9.09e-02	2.67e-04	5.22e-05	1.64e-02	7.90e-03	1.88e-03	2.16e-02	6.31e-03	2.71e-03	1.27e-02	4.47e-03	9.37e-03	3.58e-01	8.15e-03	8.02e-02	2.04e-02	7.98e-02	4.80e-01	2.19e-01	3.13e-03	9.95e-02	1.16e+00	3.26e-02
9.0	-3.5	-2.997	-4.3	8.15	8.5	2.70e-01	nan	nan	4.35e-02	2.21e-03	2.39e-02	nan	nan	8.78e-07	2.64e-02	nan	2.05e-04	9.04e-03	5.14e-01	8.09e-07	1.85e-07	3.03e-01	1.31e-01	1.47e-03	nan	6.67e-06	1.36e-01	
6.0	-2.5	-1.997	-3.8	8.85	5.5	1.66e-01	nan	nan	4.51e-07	6.69e-02	6.34e-03	2.65e-02	1.42e-07	nan	4.23e-05	2.51e-01	nan	2.14e-02	1.02e-02	8.28e-01	7.47e-05	3.10e-05	2.07e+00	1.01e+00	1.70e-02	3.82e-05	5.54e-03	5.92e-02

Notes. Columns (1)–(6): the input parameters for the MAPPINGS V models of the AGN (see Section 2). Columns (7)–(29): the predicted emission-line intensities (normalized by the corresponding H β emission) for the different AGN models.

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Table A2
The Modeling Results for the Radiative Shocks

n_{H} (1)	v_s (2)	η_{M} (3)	Abundance (4)	Fe II	Fe VIII	Mg VII	Mg V	Ar II	Na III		Ne VI	Fe VII	Ar V	Ar III	Fe VII	S IV		Ne II	Ar V	Ne V	Ne III	S III	Ar III	Ne V	O IV	Fe II
				5.34 μm (5)	5.45 μm (6)	5.50 μm (7)	5.61 μm (8)	6.99 μm (9)	7.32 μm (10)	Pf α (11)	7.65 μm (12)	7.82 μm (13)	7.90 μm (14)	8.99 μm (15)	9.53 μm (16)	10.51 μm (17)	H α (18)	12.81 μm (19)	13.10 μm (20)	14.32 μm (21)	15.56 μm (22)	18.71 μm (23)	21.83 μm (24)	24.32 μm (25)	25.89 μm (26)	25.99 μm (27)
10000.0	1000.0	0.0001	8.15	4.32e +02	1.17e +02	2.18e +02	5.19e +01	2.65e +02	2.59e +01	1.14e +02	1.28e +03	3.90e +01	1.49e +01	1.01e +02	1.17e +02	3.00e +01	4.18e +01	1.95e +03	1.58e +01	4.03e +02	1.82e +03	4.93e +02	3.54e +00	2.44e +02	5.12e +02	2.19e +02
10000.0	100.0	0.0001	8.15	1.43e +00	0.00e +00	0.00e +00	2.24e 05	2.58e 01	4.15e 03	2.32e 01	0.00e +00	6.59e 05	4.86e 04	7.37e 02	1.63e 04	3.55e 02	8.54e 02	3.11e +00	2.99e 04	3.19e 04	3.33e 01	7.06e 02	3.23e 03	9.97e 05	2.99e 02	1.24e +00
10000.0	150.0	0.0001	8.15	2.88e +00	3.86e 02	1.97e 04	1.37e 01	8.76e 01	2.05e 02	9.10e 01	3.01e 01	3.54e 02	4.71e 02	2.88e 01	9.67e 02	1.51e 01	3.40e 01	8.88e +00	3.39e 02	4.63e 01	1.97e +00	3.66e 01	1.41e 02	2.37e 01	5.58e 01	2.56e +00
10000.0	200.0	0.0001	8.15	6.65e +00	1.69e +00	5.66e 01	7.17e 01	2.12e +00	1.12e 01	2.22e +00	1.11e +01	1.54e 01	1.04e 01	1.05e +00	4.12e 01	5.58e 01	8.29e 01	2.55e +01	6.38e 02	1.86e +00	8.11e +00	1.44e +00	4.86e 02	9.38e 01	1.17e +00	6.50e +00
10000.0	25.0	0.0001	8.15	1.50e +00	0.00e +00	0.00e +00	0.00e +00	8.11e 04	0.00e +00	2.14e 03	0.00e +00	0.00e +00	0.00e +00	4.58e 08	0.00e +00	0.00e +00	7.98e 04	9.66e 03	0.00e +00	0.00e +00	0.00e +00	2.50e 05	0.00e +00	0.00e +00	0.00e +00	8.77e 01
10000.0	300.0	0.0001	8.15	2.51e +01	5.99e +00	3.89e +00	1.92e +00	1.13e +01	7.99e 01	7.14e +00	2.17e +01	4.29e 01	7.12e 01	3.90e +00	1.16e +00	1.07e +01	2.66e +00	1.05e +02	6.49e 01	5.84e +00	4.62e +01	1.21e +01	1.57e 01	2.47e +00	2.19e +01	2.95e +01
10000.0	400.0	0.0001	8.15	1.10e +02	8.84e +00	5.82e +00	8.48e +00	5.33e +01	2.34e +00	1.60e +01	3.80e +01	1.83e +00	4.33e +00	8.02e +00	5.50e +00	3.61e +01	5.97e +02	3.67e +00	4.43e +00	3.51e +01	1.21e +02	5.62e +01	2.94e 01	1.78e +01	8.35e +01	1.33e +02
10000.0	50.0	0.0001	8.15	5.56e 01	0.00e +00	0.00e +00	0.00e +00	1.30e 02	0.00e +00	1.53e 02	0.00e +00	0.00e +00	0.00e +00	7.00e 06	0.00e +00	0.00e +00	5.40e 03	1.41e 02	0.00e +00	0.00e +00	2.98e 07	6.45e 04	2.82e 07	0.00e +00	0.00e +00	4.64e 01
10000.0	600.0	0.0001	8.15	4.51e +02	1.86e +01	2.57e +01	2.79e +01	2.72e +02	9.04e +00	4.40e +01	2.56e +02	9.05e +00	1.80e +01	2.32e +01	2.82e +01	4.02e +01	1.64e +03	2.30e +01	1.92e +01	1.77e +02	6.32e +02	2.68e +02	8.61e 01	1.02e +02	2.16e +02	5.18e +02
10000.0	75.0	0.0001	8.15	6.11e 01	0.00e +00	0.00e +00	0.00e +00	4.94e 02	1.27e 05	8.48e 02	0.00e +00	0.00e +00	0.00e +00	8.74e 04	0.00e +00	1.31e 05	3.06e 02	1.81e 01	0.00e +00	0.00e +00	1.13e 04	1.76e 03	2.46e 05	0.00e +00	0.00e +00	5.66e 01

Note. Columns (1)–(4): the input parameters for the MAPPINGS V models of radiative shocks (see Section 4.1.2). Columns (5)–(27): the predicted emission-line intensities (normalized by the corresponding H β emission) for the different radiative shock models.

(This table is available in its entirety in machine-readable form in the [online article](#).)

Table A3
The Modeling Results for Star-forming Regions

U	Abundance	P/k	Fe II 5.34 μm	Fe VIII 5.45 μm	Mg VII 5.50 μm	Mg V 5.61 μm	Ar II 6.99 μm	Na III 7.32 μm	Pf α	Ne VI 7.65 μm	Fe VII 7.82 μm	Ar V 7.90 μm	Ar III 8.99 μm	Fe VII 9.53 μm	S IV 10.51 μm	H α	Ne II 12.81 μm	Ar V 13.10 μm	Ne V 14.32 μm	Ne III 15.56 μm	S III 18.71 μm	Ar III 21.83 μm	Ne V 24.32 μm	O IV 25.89 μm	Fe II 25.99 μm
(1)	(2)	(3)	(4)	(5)	(6)	(7)	(8)	(9)	(10)	(11)	(12)	(13)	(14)	(15)	(16)	(17)	(18)	(19)	(20)	(21)	(22)	(23)	(24)	(25)	(26)
-2.3	8.997	6.0	7.92e-03	nan	nan	nan	7.73e-03	2.52e-03	3.21e-02	nan	nan	1.20e-07	2.90e-01	nan	4.52e-01	1.25e-02	4.44e-01	2.41e-07	nan	1.65e+00	1.26e+00	1.87e-02	nan	1.29e-03	3.00e-03
-2.8	8.632	7.5	1.19e-02	nan	nan	1.63e-07	4.60e-03	2.64e-03	2.55e-02	nan	nan	1.31e-05	1.67e-01	nan	1.35e-01	9.71e-03	1.94e-01	2.05e-05	7.33e-06	1.03e+00	6.27e-01	1.09e-02	6.35e-06	2.00e-02	4.95e-03
-3.8	8.943	6.0	9.54e-02	nan	nan	nan	6.87e-02	3.81e-04	2.96e-02	nan	nan	nan	1.56e-01	nan	2.45e-03	1.14e-02	1.18e+00	nan	nan	3.27e-01	7.69e-01	1.02e-02	nan	2.39e-06	3.59e-02
-2.3	8.427	6.0	7.36e-03	nan	nan	6.73e-06	1.04e-03	2.94e-03	2.54e-02	nan	nan	2.00e-04	9.75e-02	3.51e-07	3.89e-01	9.73e-03	4.18e-02	3.47e-04	9.64e-05	8.33e-01	3.35e-01	6.63e-03	1.18e-04	6.94e-02	2.53e-03
-1.8	8.427	5.5	3.40e-03	nan	nan	4.98e-05	4.50e-04	3.20e-03	2.57e-02	2.44e-07	1.19e-06	8.32e-04	6.75e-02	4.29e-06	8.73e-01	9.84e-03	1.83e-02	1.43e-03	4.98e-04	8.71e-01	2.63e-01	4.60e-03	6.12e-04	1.00e-01	1.17e-03
-1.3	8.632	7.0	1.81e-03	nan	nan	8.83e-05	4.82e-04	4.04e-03	2.60e-02	1.20e-06	3.57e-06	1.96e-03	8.15e-02	1.30e-05	1.80e+00	9.93e-03	2.33e-02	3.29e-03	1.64e-04	1.32e+00	4.05e-01	5.42e-03	1.81e-03	1.23e-01	6.85e-04
-4.3	8.76	8.5	2.58e-02	nan	nan	nan	8.27e-02	4.03e-04	2.52e-02	nan	nan	nan	6.33e-02	nan	1.25e-04	9.58e-03	1.05e+00	nan	nan	1.74e-01	1.57e-01	3.34e-03	nan	2.37e-07	1.78e-02
-3.3	8.76	6.0	4.80e-02	nan	nan	nan	1.76e-02	1.38e-03	2.76e-02	nan	nan	2.09e-07	1.89e-01	nan	2.78e-02	1.06e-02	5.38e-01	3.77e-07	1.24e-07	7.88e-01	7.12e-01	1.27e-02	1.51e-07	2.68e-03	1.71e-02
-4.3	8.427	8.0	7.33e-02	nan	nan	nan	3.84e-02	5.42e-04	2.49e-02	nan	nan	nan	4.39e-02	nan	1.31e-04	9.46e-03	5.32e-01	nan	nan	1.63e-01	1.34e-01	2.74e-03	nan	1.04e-06	3.62e-02
-2.3	8.632	8.5	1.12e-03	nan	nan	2.38e-06	1.80e-03	3.57e-03	2.44e-02	nan	nan	1.85e-04	1.41e-01	nan	2.58e-01	9.22e-03	8.55e-02	1.56e-04	3.85e-05	1.07e+00	2.29e-01	7.40e-03	1.23e-05	1.21e-02	7.36e-04

Note. Columns (1)–(3): The input parameters for MAPPINGS V models of SF regions (see Section 4.2). Columns (4)–(26): The predicted emission-line intensities (normalized by the corresponding H β emission) for the different SF models.

(This table is available in its entirety in machine-readable form in the [online article](#).)

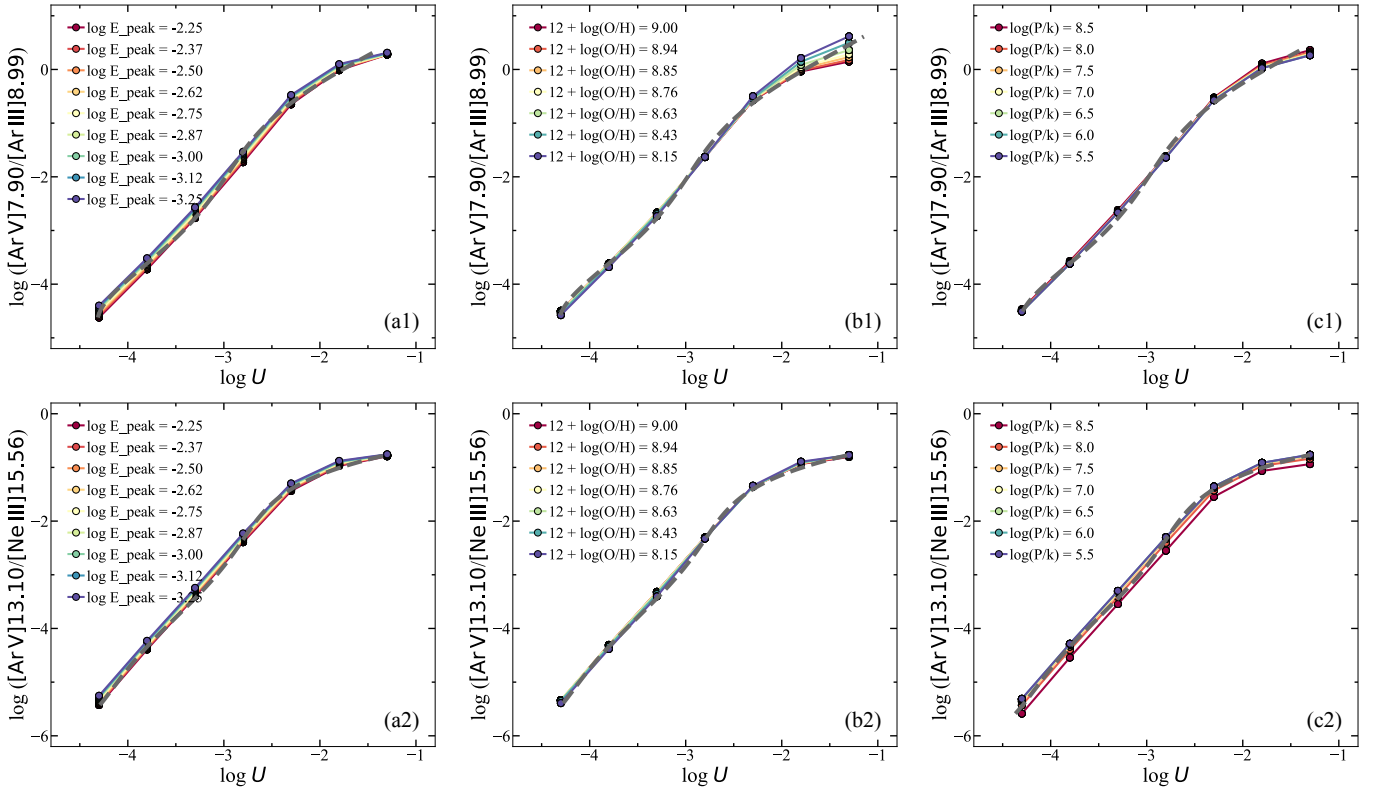


Figure A1. Same as Figure 2 but for low-luminosity AGN. Each panel, if not specifically marked, displays model results under the same parameter constraints as in Figure 2 for $\log U$ (i.e., -2.8), $12 + \log(\text{O}/\text{H})$ (i.e., 8.76), and $\log(P/k)$ (i.e., 7.0), but with a different value of $\log E_{\text{peak}}$ (-2.75 here).

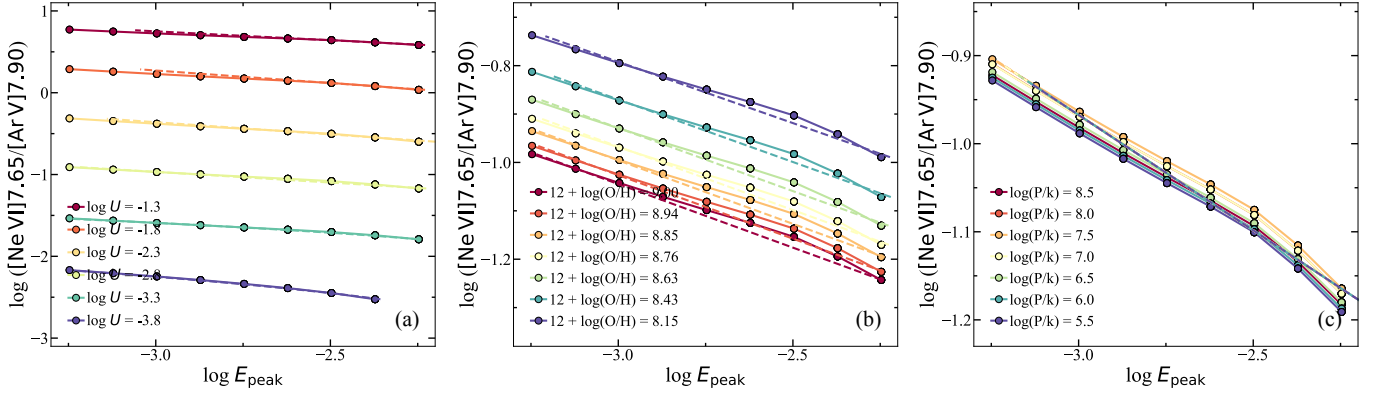


Figure A2. Same as Figure 3 but for low-luminosity AGN. Each panel, if not specifically marked, displays model results under the same parameter constraints as in Figure 3 for $\log U$ (i.e., -2.8), $12 + \log(\text{O}/\text{H})$ (i.e., 8.76), and $\log(P/k)$ (i.e., 7.0), but with a different value of $\log E_{\text{peak}}$ (-2.75 here).

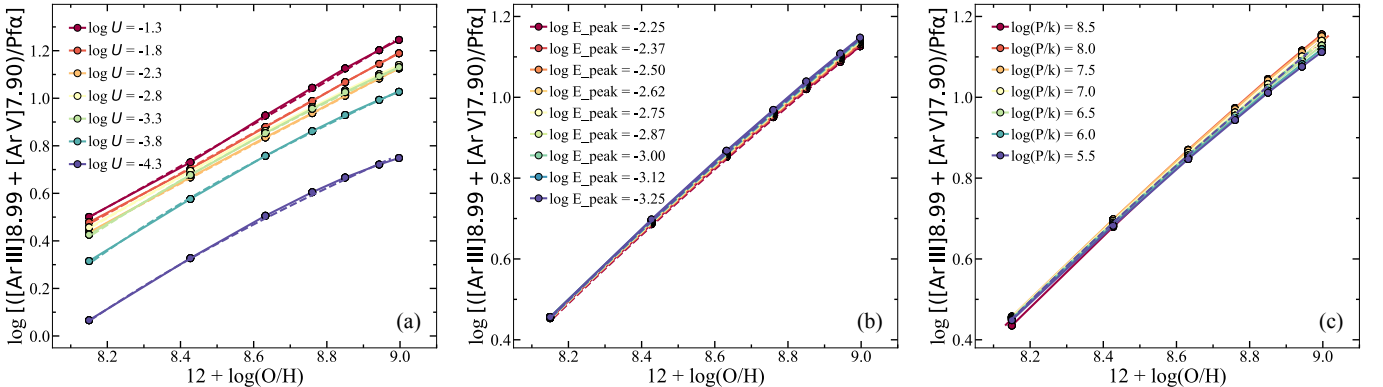


Figure A3. Same as Figure 4 but for low-luminosity AGN. Each panel, if not specifically marked, displays model results under the same parameter constraints as in Figure 4 for $\log U$ (i.e., -2.8), $12 + \log(\text{O}/\text{H})$ (i.e., 8.76), and $\log(P/k)$ (i.e., 7.0), but with a different value of $\log E_{\text{peak}}$ (-2.75 here).

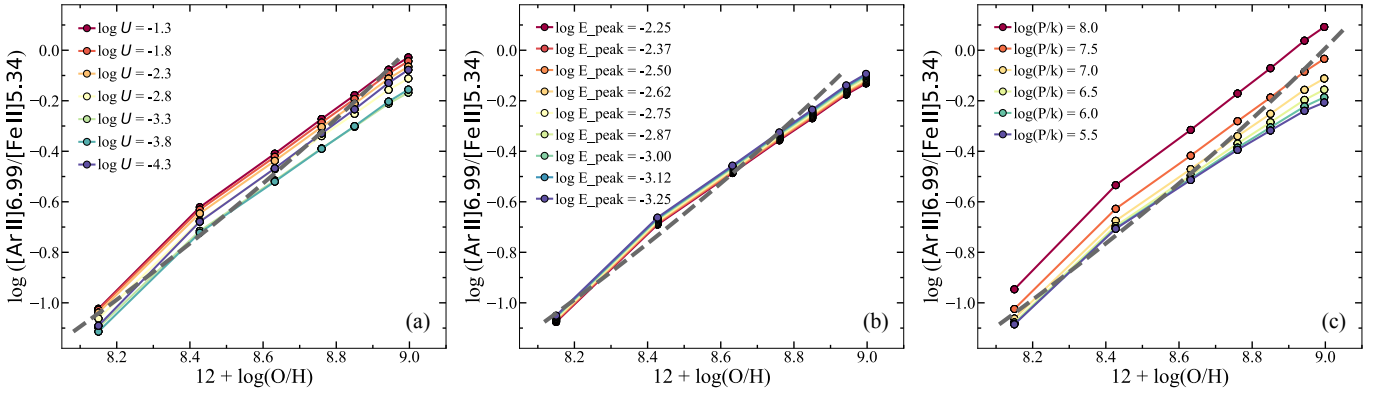


Figure A4. Same as Figure 5 but for low-luminosity AGN. Each panel, if not specifically marked, displays model results under the same parameter constraints as in Figure 5 for $\log U$ (i.e., -2.8), $12 + \log(\text{O}/\text{H})$ (i.e., 8.76), and $\log(P/k)$ (i.e., 7.0), but with a different value of $\log E_{\text{peak}}$ (-2.75 here).

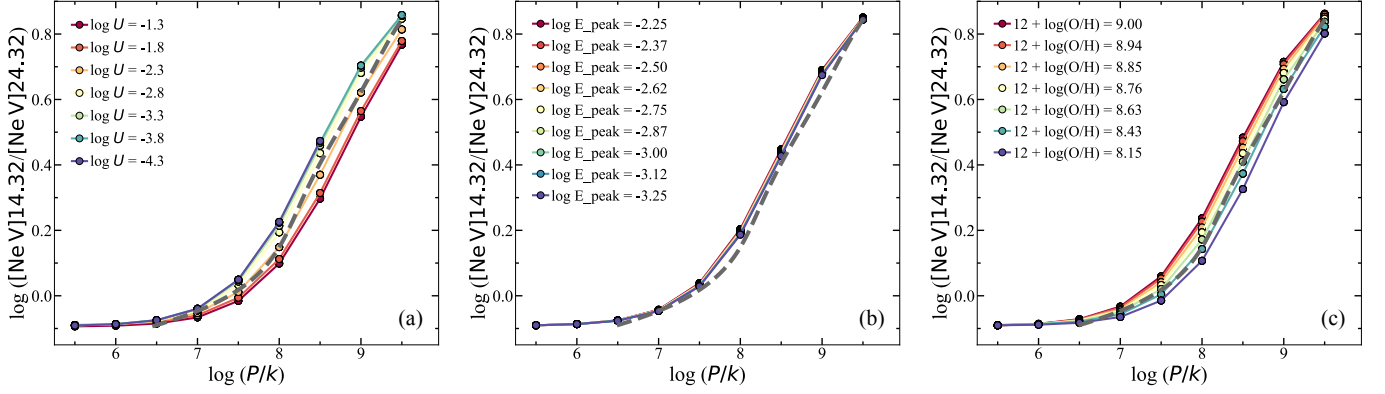


Figure A5. Same as Figure 6 but for low-luminosity AGN. Each panel, if not specifically marked, displays model results under the same parameter constraints as in Figure 6 for $\log U$ (i.e., -2.8), $12 + \log(\text{O}/\text{H})$ (i.e., 8.76), and $\log(P/k)$ (i.e., 7.0), but with a different value of $\log E_{\text{peak}}$ (-2.75 here).

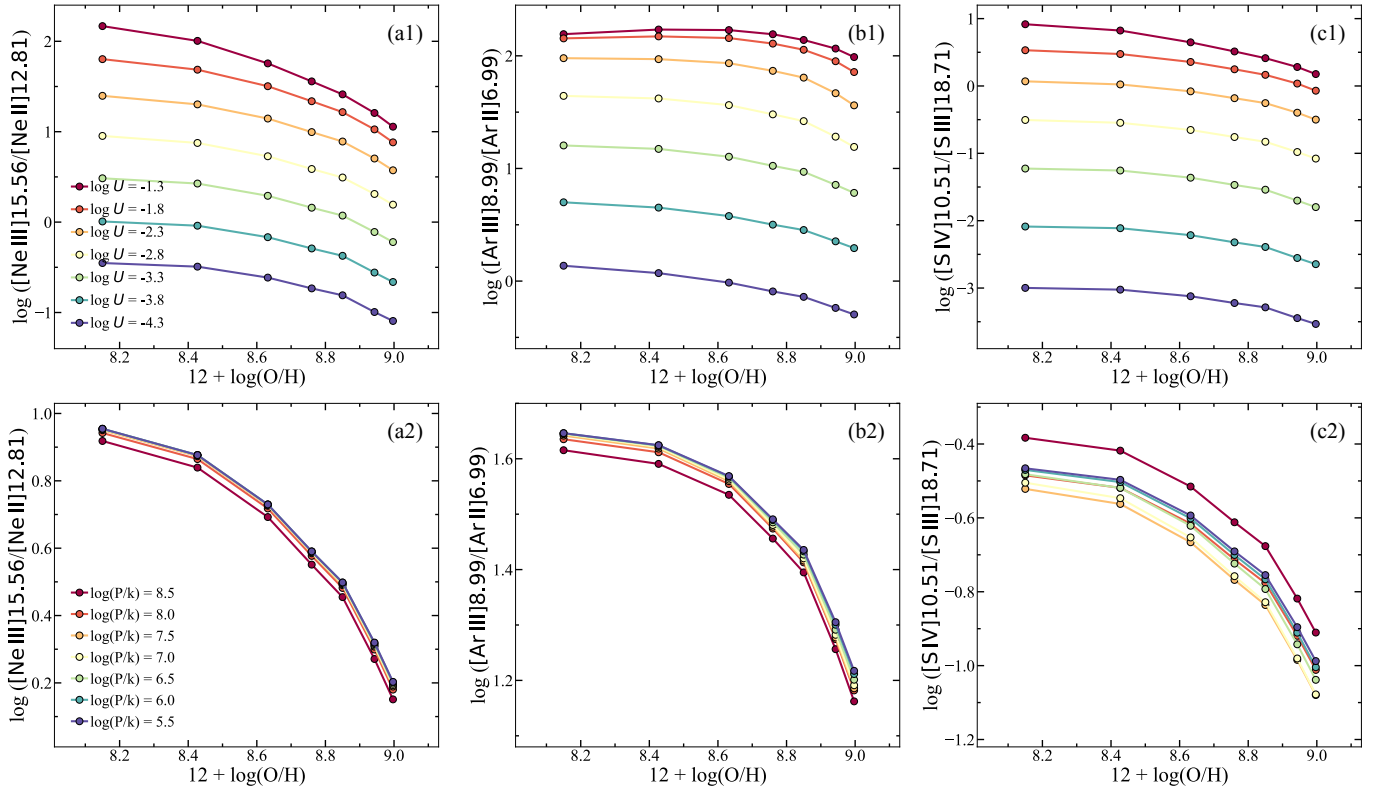


Figure A6. Dependence of (a1 and a2) $[\text{Ne III}] 15.56 \mu\text{m}/[\text{Ne II}] 12.81 \mu\text{m}$; (b1 and b2) $[\text{Ar III}] 8.99 \mu\text{m}/[\text{Ar II}] 6.99 \mu\text{m}$; and (c1 and c2) $[\text{S IV}] 10.51 \mu\text{m}/[\text{S III}] 18.71 \mu\text{m}$ on the metallicity ($12 + \log(\text{O}/\text{H})$), as predicted by the SF photoionization models (colored points) discussed in Section 4.2. The top and bottom panels display model results under specific constraints on $\log(P/k)$ (i.e., 7.0) and $\log U$ (i.e., -2.8), respectively.

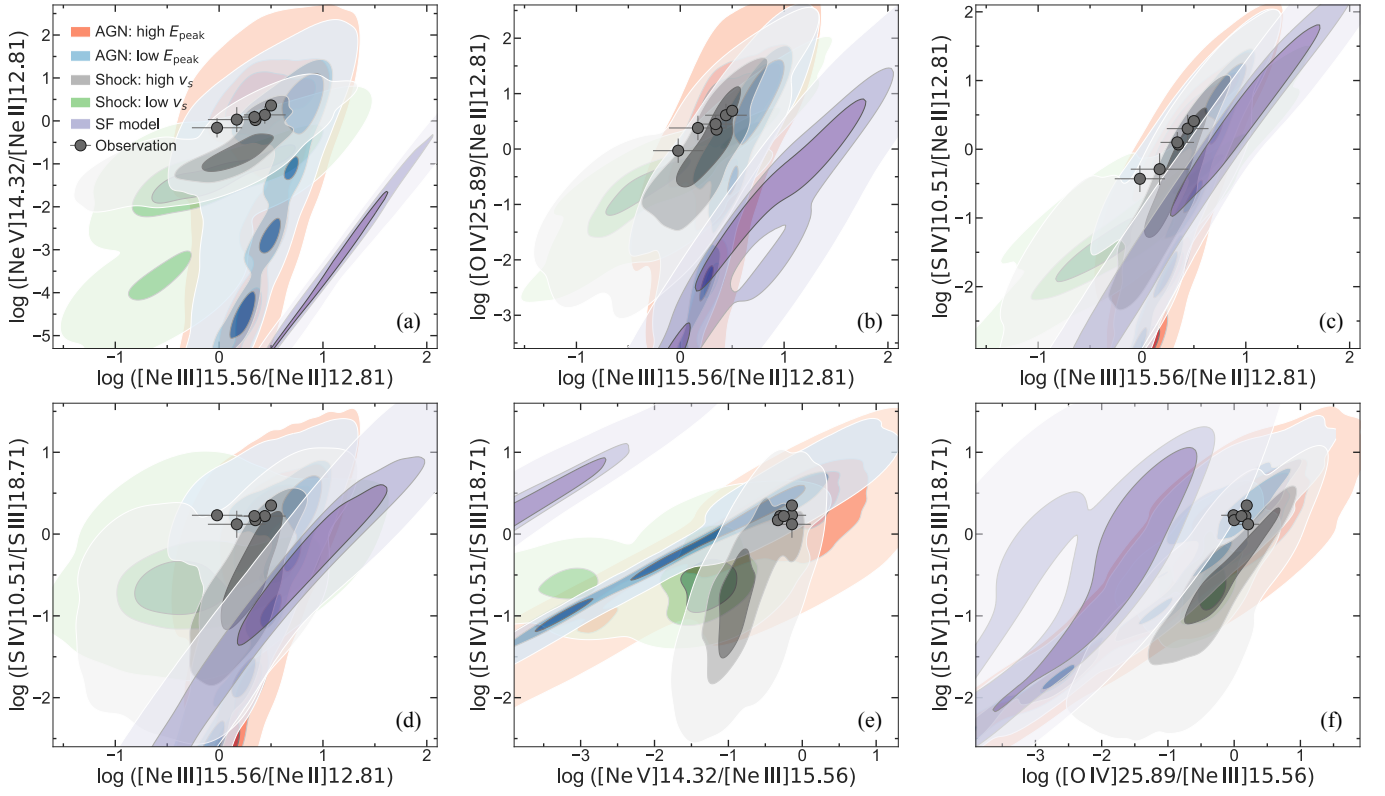


Figure A7. The same as Figure 11, but with added contours for the SF photoionization models discussed in Section 4.2. Measurements for the central $r = 0''.75$ regions of six Seyferts represented by the six gray points are taken from L. Zhang et al. (2024b).

Table A4

Coefficients of the Best-fit Correlations for U of the Active Galactic Nuclei with $R = [\text{Ar V}] 7.90 \mu\text{m}/[\text{Ar III}] 8.99 \mu\text{m}$, $[\text{Ar V}] 13.10 \mu\text{m}/[\text{Ne III}] 15.56 \mu\text{m}$, and $[\text{Ar V}] 7.90 \mu\text{m}/[\text{Ne III}] 15.56 \mu\text{m}$

R	$[\text{Ar V}] 7.90 \mu\text{m}/$ $[\text{Ar III}] 8.99 \mu\text{m}$	$[\text{Ar V}] 13.10 \mu\text{m}/$ $[\text{Ne III}] 15.56 \mu\text{m}$	$[\text{Ar V}] 7.90 \mu\text{m}/$ $[\text{Ne III}] 15.56 \mu\text{m}$	$[\text{Ar V}] 7.90 \mu\text{m}/$ $[\text{Ar III}] 8.99 \mu\text{m}$	$[\text{Ar V}] 13.10 \mu\text{m}/$ $[\text{Ne III}] 15.56 \mu\text{m}$	$[\text{Ar V}] 7.90 \mu\text{m}/$ $[\text{Ne III}] 15.56 \mu\text{m}$
$\log E_{\text{peak}}$	$[-2.0, -0.95]$	$[-2.0, -0.95]$	$[-2.0, -0.95]$	$[-3.25, -2.25]$	$[-3.25, -2.25]$	$[-3.25, -2.25]$
c_5	$-4.525e-03$	$3.576e-03$	$7.195e-03$	$-5.677e-03$	$8.764e-03$	$1.533e-02$
c_4	$-3.193e-02$	$7.535e-02$	$1.373e-01$	$-5.021e-02$	$1.642e-01$	$2.772e-01$
c_3	$-3.924e-03$	$5.996e-01$	$1.009e+00$	$-1.013e-01$	$1.173e+00$	$1.922e+00$
c_2	$3.291e-01$	$2.216e+00$	$3.524e+00$	$1.350e-01$	$3.958e+00$	$6.353e+00$
c_1	$1.022e+00$	$4.165e+00$	$6.193e+00$	$9.735e-01$	$3.958e+00$	$1.043e+01$
c_0	$-1.993e+00$	$3.979e-01$	$1.685e+00$	$-1.762e+00$	$3.958e+00$	$4.295e+00$
RMS scatter	0.16 dex	0.17 dex	0.16 dex	0.10 dex	0.10 dex	0.07 dex

Note. Coefficients in Equation (1).

Table A5
Coefficients of the Best-fit Correlations for E_{peak} for the Active Galactic Nuclei with $R = [\text{Ne VI}] 7.65 \mu\text{m}/[\text{Ar V}] 7.90 \mu\text{m}$

$\log E_{\text{peak}}$	[-2.0, -0.95]					[-3.25, -2.25]				
$\log U$	[-3.8, -3.3]	[-3.3, -2.8]	[-2.8, -2.3]	[-2.3, -1.8]	[-1.8, -1.3]	[-3.8, -3.3]	[-3.3, -2.8]	[-2.8, -2.3]	[-2.3, -1.8]	[-1.8, -1.3]
$a_{Z,2}$	$2.328e-02$	$-6.770e-03$	$3.188e-03$	$2.589e-02$	$1.201e-01$	$-3.461e+00$	$2.693e-04$	$-6.189e-06$	$1.904e-04$	$9.298e-02$
$a_{Z,1}$	$-3.564e-01$	$1.201e-01$	$-8.139e-02$	$-5.474e-01$	$-2.344e+00$	$6.260e+01$	$-4.837e-03$	$-3.189e-03$	$-5.130e-03$	$-2.174e+00$
$a_{U,1}$	$-6.036e-01$	$-2.726e-01$	$1.671e-02$	$2.721e-02$	$3.613e-02$	$-5.197e+00$	$-3.382e-04$	$-5.607e-03$	$-9.945e-05$	$1.452e-01$
a_0	$-3.804e-01$	$-1.163e+00$	$6.438e-01$	$3.052e+00$	$1.175e+01$	$-3.047e+02$	$2.612e-02$	$3.733e-02$	$3.331e-02$	$1.249e+01$
$b_{Z,2}$	$-1.814e-01$	$-2.021e-01$	$-2.144e-01$	$-3.855e-01$	$-3.609e-01$	$-1.523e-01$	$8.256e-02$	$-2.629e-01$	$3.154e+00$	$-6.706e-01$
$b_{Z,1}$	$3.207e+00$	$3.450e+00$	$3.203e+00$	$5.701e+00$	$5.470e+00$	$2.186e+00$	$-2.568e+00$	$4.522e+00$	$6.398e+00$	$1.392e+01$
$b_{U,1}$	$8.213e-01$	$-5.776e-01$	$1.167e+00$	$4.948e-01$	$1.353e-01$	$1.696e+00$	$6.858e+00$	$8.318e-01$	$-2.817e+00$	$2.158e+00$
b_0	$-1.381e+01$	$-1.900e+01$	$-1.106e+01$	$-2.076e+01$	$-2.027e+01$	$-3.953e+00$	$3.908e+02$	$5.906e+01$	$2.121e+02$	$-6.115e+01$
$c_{Z,2}$	$-7.294e-02$	$-2.031e-02$	$-6.264e-02$	$-9.451e-02$	$-3.524e-02$	$2.312e-01$	$-3.484e+01$	$1.071e+00$	$4.126e+01$	$1.183e+01$
$c_{Z,1}$	$1.337e+00$	$4.443e-01$	$1.068e+00$	$1.483e+00$	$5.172e-01$	$-3.530e+00$	$6.288e+02$	$2.125e-02$	$-4.495e+02$	$-2.008e+02$
$c_{U,1}$	$-1.940e-01$	$-4.896e-01$	$-7.116e-02$	$-4.659e-01$	$-5.835e-01$	$3.316e-01$	$2.094e+01$	$3.466e+01$	$3.992e+01$	$-9.069e+00$
c_0	$-8.895e+00$	$-6.098e+00$	$-7.158e+00$	$-9.052e+00$	$-4.978e+00$	$1.244e+01$	$-3.459e+03$	$-1.348e+02$	$-6.133e-02$	$8.230e+02$
RMS scatter	0.05 dex	0.03 dex	0.02 dex	0.02 dex	0.03 dex	0.02 dex	0.04 dex	0.06 dex	0.10 dex	0.13 dex

Note. Coefficients in Equation (2) for different ranges of $\log U$.

Table A6
Coefficients in the Best-fit Correlations for $12 + \log(\text{O}/\text{H})$ for the Active Galactic Nuclei with $R = ([\text{Ar III}] 8.99 \mu\text{m} + [\text{Ar V}] 7.90 \mu\text{m})/\text{Pfc}\alpha$

$\log E_{\text{peak}}$	[-2.0, -0.95]						[-3.25, -2.25]					
$\log U$	[-4.3, -3.8]	[-3.8, -3.3]	[-3.3, -2.8]	[-2.8, -2.3]	[-2.3, -1.8]	[-1.8, -1.3]	[-4.3, -3.8]	[-3.8, -3.3]	[-3.3, -2.8]	[-2.8, -2.3]	[-2.3, -1.8]	[-1.8, -1.3]
$a_{E,3}$	-1.179e-01	-1.615e-02	-4.535e-03	-4.274e-02	-4.723e-04	-7.667e-03	-4.523e-02	-2.561e-02	-1.327e-03	5.427e-05	-9.078e-07	-1.111e-02
$a_{E,2}$	-4.574e-01	-4.859e-02	-3.221e-03	-2.237e-01	-2.183e-03	-3.959e-02	-2.732e-01	-1.594e-01	-1.143e-02	4.498e-04	-1.428e-05	-1.223e-01
$a_{E,1}$	-5.220e-01	-2.267e-02	2.951e-02	-3.476e-01	-5.951e-06	-6.117e-02	-3.843e-01	-2.474e-01	-3.264e-02	1.361e-03	-4.716e-05	-4.725e-01
$a_{U,1}$	3.616e-02	4.227e-02	4.429e-02	1.898e-02	3.553e-05	-9.674e-03	3.101e-02	1.375e-02	-1.684e-01	-2.234e-01	4.427e-04	-3.569e-04
a_0	1.804e-01	3.178e-01	3.141e-01	1.571e-02	9.976e-03	9.590e-03	5.625e-01	3.154e-01	-3.461e-01	-4.717e-01	3.840e-03	-6.767e-01
$b_{E,3}$	-1.482e+00	-1.597e-02	1.435e-01	-8.123e-01	4.264e+00	-1.074e+00	-5.291e-01	-4.076e-01	-1.391e-01	-1.549e-01	3.267e-01	3.691e-01
$b_{E,2}$	-6.125e+00	2.944e-02	6.347e-01	-5.457e+00	-3.372e+00	-5.066e+00	-4.069e+00	-3.051e+00	-1.192e+00	-1.326e+00	1.508e+00	4.293e+00
$b_{E,1}$	-7.469e+00	7.895e-01	1.560e+00	-9.141e+00	1.286e+01	-6.051e+00	-1.001e+01	-7.203e+00	-3.453e+00	-3.862e+00	3.514e+00	8.758e+00
$b_{U,1}$	1.122e+00	1.085e+00	1.001e+00	6.683e-01	4.292e+00	-1.833e-01	7.654e-01	2.453e-01	-2.903e+00	-2.203e+01	4.718e+01	-7.299e-01
b_0	-1.360e-01	2.056e+00	1.454e+00	-5.911e+00	-3.485e+01	-1.087e+01	-5.733e+00	-5.770e+00	-1.466e+01	-6.875e+01	-9.986e+01	7.193e+00
$c_{E,3}$	-7.811e-01	1.094e-01	1.644e-01	-3.626e-01	1.475e+00	-7.442e-01	-3.195e-01	-2.500e-01	-1.247e-01	-1.685e-01	4.815e-01	1.715e-01
$c_{E,2}$	-3.303e+00	3.700e-01	4.818e-01	-2.883e+00	-6.043e+00	-2.681e+00	-2.456e+00	-1.880e+00	-1.064e+00	-1.440e+00	2.829e+00	2.334e+00
$c_{E,1}$	-3.998e+00	8.657e-01	8.866e-01	-5.002e+00	5.641e+00	-1.566e+00	-6.055e+00	-4.498e+00	-3.084e+00	-4.190e+00	7.403e+00	5.039e+00
$c_{U,1}$	4.894e-01	4.223e-01	4.056e-01	2.927e-01	4.397e+00	8.821e-01	2.132e-01	-1.263e-02	-1.898e+00	-1.340e+01	3.847e+01	-9.073e-01
c_0	7.766e+00	8.946e+00	8.508e+00	4.663e+00	-3.983e+00	5.523e+00	3.710e+00	3.877e+00	-2.217e+00	-3.560e+01	-2.531e+01	1.165e+01
rms scatter	0.02 dex	0.01 dex	0.01 dex	0.01 dex	0.01 dex	0.01 dex	0.02 dex	0.01 dex	0.01 dex	0.02 dex	0.02 dex	0.02 dex

Note. Coefficients in Equation (6) for different ranges of $\log U$.

Table A7Coefficients of the Best-fit Correlations for $12 + \log(\text{O}/\text{H})$ for the Active Galactic Nuclei with $R = [\text{Ar II}] 6.99 \mu\text{m}/[\text{Fe II}] 5.34 \mu\text{m}$, $[\text{Ne II}] 12.81 \mu\text{m}/[\text{Fe II}] 5.34 \mu\text{m}$ $[\text{Ar II}] 6.99 \mu\text{m}/[\text{Fe II}] 25.99 \mu\text{m}$, and $[\text{Ne II}] 12.81 \mu\text{m}/[\text{Fe II}] 25.99 \mu\text{m}$

	$[\text{Ar II}]/[\text{Fe II}]$	$[\text{Ar II}]/[\text{Fe II}]$	$[\text{Ne II}]/[\text{Fe II}]$	$[\text{Ne II}]/[\text{Fe II}]$	$[\text{Ar II}]/[\text{Fe II}]$	$[\text{Ar II}]/[\text{Fe II}]$	$[\text{Ne II}]/[\text{Fe II}]$	$[\text{Ne II}]/[\text{Fe II}]$
R	$5.34 \mu\text{m}$	$5.34 \mu\text{m}$	$5.34 \mu\text{m}$	$5.34 \mu\text{m}$	$25.99 \mu\text{m}$	$25.99 \mu\text{m}$	$25.99 \mu\text{m}$	$25.99 \mu\text{m}$
$\log E_{\text{peak}}$	$[-2.0, -0.95]$	$[-3.25, -2.25]$	$[-2.0, -0.95]$	$[-3.25, -2.25]$	$[-2.0, -0.95]$	$[-3.25, -2.25]$	$[-2.0, -0.95]$	$[-3.25, -2.25]$
c_2	$-7.021e-02$	$-1.217e-01$	$-6.849e-02$	$-4.032e-02$	$1.910e-01$	$1.794e-01$	$1.973e-01$	$2.056e-01$
c_1	$7.508e-01$	$6.842e-01$	$8.979e-01$	$8.627e-01$	$9.507e-01$	$9.507e-01$	$5.772e-01$	$5.243e-01$
c_0	$9.007e+00$	$8.994e+00$	$8.198e+00$	$8.154e+00$	$8.661e+00$	$8.668e+00$	$7.906e+00$	$7.894e+00$
rms scatter	0.08 dex	0.08 dex	0.07 dex	0.07 dex	0.05 dex	0.05 dex	0.05 dex	0.04 dex

Note. Coefficients in Equation (10).**Table A8**Coefficients of the Best-fit Correlations for P/k for the Active Galactic Nuclei with $R = [\text{Ne V}] 14.32 \mu\text{m}/[\text{Ne V}] 24.32 \mu\text{m}$

$\log E_{\text{peak}}$	$[-2.0, -0.95]$	$[-3.25, -2.25]$
c_5	$3.340e+01$	$2.768e+01$
c_4	$-8.183e+01$	$-6.887e+01$
c_3	$7.367e+01$	$6.377e+01$
c_2	$-2.947e+01$	$-2.662e+01$
c_1	$7.065e+00$	$6.909e+00$
c_0	$7.494e+00$	$7.384e+00$
RMS scatter	0.19 dex	0.20 dex

Note. Coefficients in Equation (11).**Table A9**Coefficients of the Best-fit Correlations for $\log U$ for Star-forming Regions with $R = [\text{S IV}] 10.51 \mu\text{m}/[\text{Ne III}] 15.56 \mu\text{m}$



















R	$[\text{S IV}] 10.51 \mu\text{m}/[\text{Ne III}] 15.56 \mu\text{m}$
c_3	$3.652e-02$
c_2	$3.357e-01$
c_1	$1.605e+00$
c_0	$-1.513e+00$
RMS scatter	0.17 dex

Note. Coefficients in Equation (12).**Table A10**Coefficients of the Best-fit Correlations for $12 + \log(\text{O}/\text{H})$ of the Star-forming Regions with $R = [\text{Ne II}] 15.56 \mu\text{m}/\text{P}\alpha$ and $[\text{Ar II}] 6.99 \mu\text{m}/\text{P}\alpha$

R	$[\text{Ne II}] 15.56 \mu\text{m}/\text{P}\alpha$	$[\text{Ne II}] 15.56 \mu\text{m}/\text{P}\alpha$	$[\text{Ne II}] 15.56 \mu\text{m}/\text{P}\alpha$	$[\text{Ar II}] 6.99 \mu\text{m}/\text{P}\alpha$	$[\text{Ar II}] 6.99 \mu\text{m}/\text{P}\alpha$	$[\text{Ar II}] 6.99 \mu\text{m}/\text{P}\alpha$
$\log U$	$[-4.3, -3.3]$	$[-3.3, -2.3]$	$[-2.3, -1.3]$	$[-4.3, -3.3]$	$[-3.3, -2.3]$	$[-2.3, -1.3]$
$a_{U,2}$	$-1.894e-04$	$1.338e-01$	$6.611e-02$	$-2.480e-01$	$1.458e-01$	$2.534e-01$
$a_{U,1}$	$-1.775e-03$	$6.566e-01$	$3.383e-01$	$-2.191e+00$	$5.631e-01$	$1.173e+00$
a_0	$-1.827e-03$	$5.575e-01$	$1.836e-01$	$-4.840e+00$	$-3.860e-02$	$7.948e-01$
$b_{U,2}$	$-2.126e+00$	$2.059e+00$	$7.611e-01$	$3.641e+02$	$7.973e-01$	$7.452e-01$
$b_{U,1}$	$2.271e+01$	$9.311e+00$	$2.590e+00$	$2.577e+03$	$2.991e+00$	$2.490e+00$
b_0	$-1.339e+02$	$1.245e+01$	$3.864e+00$	$4.540e+03$	$2.317e+00$	$1.440e+00$
$c_{U,2}$	$-2.601e-03$	$1.138e+00$	$1.120e-01$	$2.030e+02$	$3.618e-01$	$7.675e-02$
$c_{U,1}$	$6.382e+01$	$5.502e+00$	$3.958e-01$	$1.438e+03$	$1.755e+00$	$3.242e-01$
c_0	$1.123e+02$	$1.576e+01$	$9.442e+00$	$2.543e+03$	$1.114e+01$	$9.355e+00$
RMS scatter	0.03 dex	0.02 dex	0.01 dex	0.03 dex	0.02 dex	0.02 dex

Note. Coefficients in Equation (13) for different ranges of $\log U$.

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