

Physical and chemical conditions of molecular gas in NGC 1068

The nuclear feedback in the circumnuclear disk and starburst ring

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ABSTRACT

Context. Molecular gas in galaxies is shaped by both star formation and active galactic nuclei. In NGC 1068, the circumnuclear disk and the starburst ring offer a nearby case to study these effects with many molecular tracers. Earlier work has shown strong outflow activity and complex chemistry, which motivates the use of methods that combine radiative transfer with time-dependent chemistry.

Aims. Our aim is to map the physical conditions across the circumnuclear disk and the starburst ring of NGC 1068 and to test whether the nuclear outflow influences the molecular gas in the ring. We also examine whether the heating or the quiescent cloud scenario better matches the observations.

Methods. We used archival ALMA observations obtained in bands 3, 4, and 5, covering molecular species including HCN, HCO⁺, HNC, CS, CN, and C₂H. All data cubes were convolved to a common resolution of 0''.8 and sampled into 56 pc hexagons with a signal-to-noise threshold of three. We performed hierarchical Bayesian inference that links a non-local thermodynamic equilibrium radiative transfer module (SpectralRadex) with chemical modeling. To make the analysis efficient, we replaced direct UCLCHEM calculations with a neural network emulator trained on a large model grid. Sampling was done with Nautilus. We also compared our results with previous studies that used RADEX and UCLCHEM for selected regions.

Results. The emulator reproduces the UCLCHEM abundances with a low error and allows inference at modest computational cost. We find clear radial and azimuthal variations in gas density, temperature, column density, and cosmic-ray ionization rate. Toward the inner edge of the starburst ring, both physical properties and CO line profiles suggest that the gas there is highly disturbed.

Conclusions. By coupling chemistry and radiative transfer within a hierarchical framework, and by using a neural network to speed up the chemical calculations, we obtained spatially resolved constraints on the physical conditions in NGC 1068. The radial gradients and the non-Gaussian CO profiles indicate that the nuclear outflow influences the inner part of the starburst ring. Observations at higher angular resolution would resolve the gas components that are blended within our 56 pc beam and clarify how the nuclear outflow disturbs the inner starburst ring.

Key words. galaxies: active – galaxies: individual: NGC 1068 – galaxies: ISM – ISM: molecules

1. Introduction

Galaxy evolution is strongly influenced by feedback processes that regulate star formation through the activity of active galactic nuclei (AGNs). The energy released by AGNs can suppress star formation by removing gas from host galaxies (negative feedback; e.g., Fabian 2012; Harrison 2017). Conversely, AGN-driven outflows can compress gas and potentially enhance star formation (positive feedback; e.g., Silk 2013; Zubovas et al. 2013). Stellar feedback, which is driven by winds and supernovae, plays a similarly important role in this cycle (Koudmani et al. 2019, 2022; Leung et al. 2019; Murthy et al. 2022). As a direct probe of these activities, sub-millimeter molecular tracers serve as a crucial tool for studying the physical conditions in galaxy centers, as most of the gas is in molecular form and is often obscured by dust. Different molecules trace distinct environments: HCO, HCO⁺, and C₂H are prominent in photon-dominated regions (PDRs; e.g., García-Burillo et al. 2002; Gerin et al. 2009; Martín et al. 2009;

García-Burillo et al. 2017; Holdship et al. 2021); HCN and CS trace dense gas clumps (e.g., Gao & Solomon 2004; Aladro et al. 2011; Scourfield et al. 2020; Li et al. 2021; Butterworth et al. 2022); and CH₃OH, HNCO, and SiO are enhanced in shocked gas (e.g., Kelly et al. 2017; Huang et al. 2022, 2023). This correspondence is not unique, however, since the same species can also trace cosmic-ray dominated regions (CRDRs), where a high ionization rate produces PDR-like chemistry deep within clouds at high visual extinction (Holdship et al. 2021).

NGC 1068 represents an archetypal system for studying the interplay between AGN and starburst activity (Romeo & Fathi 2016). Located at a distance of 14 Mpc (Bland-Hawthorn et al. 1997; 1'' ~ 70 pc), its proximity enables sufficient spatial resolution to distinguish between star formation and AGN-driven processes. Interferometric CO mapping by Schinnerer et al. (2000) revealed three principal molecular gas components: an extended starburst ring at a galactocentric radius of ~1.5 kpc, a compact circumnuclear disk (CND) extending to ~200 pc from the nucleus, and an elongated stellar bar spanning approximately 2 kpc with a position angle of ~48° (Scoville et al. 1988). The galaxy

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hosts a biconical ionized and molecular gas outflow driven by the central AGN (e.g., [Das et al. 2007](#); [García-Burillo et al. 2014](#); [Saito et al. 2022](#)). Kinematic evidence demonstrates that molecular gas has been displaced out of the galactic plane into a three-dimensional outflow geometry ([García-Burillo et al. 2019](#)). Detailed CO outflow mass rates within the CND have been calculated by [Zhang et al. \(2025\)](#), and molecular outflow signatures have been detected in bow-shock arc kinematics ([García-Burillo et al. 2014, 2019](#); [Sánchez-García et al. 2022](#)).

Despite the detailed characterization of the central outflow, the broader connection between AGN-driven outflows and star formation in the starburst ring of NGC 1068 remains unresolved. [Sánchez-García et al. \(2022\)](#) investigated the relationship between star formation rate and dense molecular gas using CO, HCN, and HCO^+ from ALMA, together with $\text{Pa}\alpha$ emission from the *Hubble Space Telescope* (HST). By assessing gas boundedness, they attributed the enhanced dense gas fractions in the bar-ring interaction region mainly to molecular gas compression caused by intense cloud-cloud collisions. However, because this interface also overlaps with the potential outflow impact zone, the contribution from AGN-driven outflows could not be fully ruled out. The limited spatial resolution of their observations further restricts the ability to distinguish between these processes. Therefore, determining whether AGN-driven outflows reach the starburst ring and influence its star formation activity remains a key open question.

Resolving this question requires looking beyond kinematics to the underlying physical conditions of the gas, where molecular chemistry offers a complementary probe. Previous surveys have already established a rich chemical baseline for the nuclear region of NGC 1068. Notably, [Viti et al. \(2014\)](#) combined ALMA and Plateau de Bure Interferometer data to characterize five chemically distinct regions within the circum-nuclear disk. Their analysis revealed a multiphase interstellar medium and demonstrated that the starburst ring exhibits lower molecular column densities than the CND, despite similarities in chemical composition. Subsequent multi-transition studies further explored these differences using dense gas and shock tracers (e.g., [Scourfield et al. 2020](#); [Huang et al. 2022](#); [Butterworth et al. 2022](#)). A common limitation in these studies is the strong degeneracy between gas density and temperature when radiative transfer or chemical modeling is applied in isolation. This highlights the need for modeling frameworks that self-consistently couple non-local thermodynamic equilibrium (non-LTE) excitation with chemistry to robustly constrain the physical conditions of molecular gas.

To overcome the degeneracies inherent to isolated radiative transfer or chemical modeling, previous studies have demonstrated that coupling non-LTE radiative transfer calculations with time-dependent chemistry provides significantly tighter constraints on gas density and temperature ([Viti 2017](#); [Harada et al. 2019](#)). However, the computational cost of such coupled modeling is substantial. To mitigate this limitation, [de Mijolla et al. \(2019\)](#) developed the first neural-network emulators designed to accelerate the inference process. Building on this approach, [Behrens et al. \(2024\)](#) recently utilized these emulators to enable robust constraints on the cosmic-ray ionization rate in the nearby starburst galaxy NGC 253. In parallel, advances in statistical methodologies have shown that hierarchical Bayesian frameworks can effectively suppress spurious parameter correlations, as demonstrated by [Tanaka et al. \(2024\)](#) for molecular gas in NGC 253.

Building on this foundation, we applied this advanced modeling framework to NGC 1068. Our goal was to examine how

AGN-driven outflows reshape the molecular content along their paths and evaluate whether they ultimately regulate star formation in the starburst ring.

This paper is organized as follows: Section 2 describes the observations and data reduction. We present the Bayesian method and neural network workflow in Section 3. Section 4 presents the model favorability, corner plots, and parameter distribution maps. In Section 5, we compare our results with previous studies and assess whether AGN-launched outflows reach the starburst ring. We summarize our findings in Section 6.

2. Observations

2.1. ALMA data

We used archival data from three ALMA programs: 2018.1.01506.S (PI: S. Viti) with Band 3 and Band 4, 2018.1.01684.S (PI: T. Tosaki) with Band 3, and 2018.1.00321.S (PI: D. Pesce) with Band 5. Table 1 lists all molecular transitions, project IDs, and synthesized beam sizes. The native beam sizes range from $0''.3$ (~ 20 pc) to $0''.8$ (~ 60 pc) at the distance of NGC 1068, which is comparable to the size of a giant molecular cloud ([Leroy et al. 2015](#)). All data were calibrated and imaged using CASA ([CASA Team et al. 2022](#)).

Since our science goal required maps that cover both the full starburst ring and the CND with comparable resolution and sensitivity, we focused on low- J transitions of common tracers well detected across both regions, including HCN, HNC, HCO^+ , CS, CN, and C_2H . These lines provide wide spatial coverage and a strong signal-to-noise, suitable for Bayesian modeling based on real detections. Although the archive includes many additional transitions, most are only bright in limited areas and are weak or undetected elsewhere. Including them would introduce numerous 3σ upper limits with little benefit for our Bayesian analysis. Thus, we restricted our study to the lines listed in Table 1.

The rest frequencies were determined using the systemic velocity from [García-Burillo et al. \(2019\)](#), with $v_{\text{sys}}(\text{HEL}) \approx 1130$ km/s. The phase tracking center was $\alpha_{2000} = 02^{\text{h}}42^{\text{m}}40.771^{\text{s}}$, $\delta_{2000} = -00^{\circ}00'47.84''$, which is the galaxy's center according to SIMBAD, taken from the Two Micron All Sky Survey (2MASS; [Skrutskie et al. \(2006\)](#)).

2.2. Region selection and moment-0 maps

We first convolved all image cubes to $0''.8$, which is the largest beam size among the datasets. The line intensity maps were integrated over selected velocity ranges to capture significant emission from both rotational and outflow motions in NGC 1068. For most transitions, we integrated fluxes within $|v - v_{\text{sys}}| \leq 230$ km s $^{-1}$ to encompass these motions ([García-Burillo et al. 2014](#)). However, some transitions required modified velocity windows: The C_2H ($N = 1-0$) line, which is denoted as C_2H ($1-0$) throughout this work, shows a complex spectral pattern consisting of six hyperfine transitions that can be separated into two distinct fine-structure groups. Since these components appear blended at our velocity resolution, we employed a broader integration window of $v - v_{\text{sys}} \in [-510, 230]$ km s $^{-1}$ to include the complete C_2H ($1-0$) transition ([García-Burillo et al. 2017](#)).

We used the HExagonal Region Averager (HERA)¹ code ([Behrens 2024](#)) to partition the integrated intensity maps into adjoining hexagonal regions, each with a characteristic size of 56 pc, equivalent to the $\sim 0''.8$ beam size. The code retains only

¹ <https://github.com/ebbehrens97/HERA>

Table 1: Observational details.

Molecule	Transition	Rest Frequency (GHz)	E_u/k (K)	Spatial Resolution	$N_{\text{Regions}} > 3\sigma$	Project ID	MRS ($''$)	RMS (mJy/beam)
C ₂ H	$N = 1-0$	87.3169	4.2	$0.''66 \times 0.''53$	64	2018.1.01506.S	6.6	0.42
HCN	$1-0$	88.6316	4.3	$0.''34 \times 0.''32$	263	2018.1.01506.S	6.6	0.42
HNC	$1-0$	90.6636	4.4	$0.''34 \times 0.''32$	214	2018.1.01506.S	6.6	0.42
HCO ⁺	$1-0$	89.1885	4.3	$0.''34 \times 0.''32$	241	2018.1.01506.S	6.6	0.42
CS	$2-1$	97.9809	7.1	$0.''78 \times 0.''45$	308	2018.1.01684.S	9.8	0.82
CN	$N = 1-0, J = 1/2-1/2$	113.1441	5.4	$0.''43 \times 0.''36$	152	2018.1.01684.S	9.8	0.46
CN	$N = 1-0, J = 3/2-1/2$	113.4910	5.4	$0.''43 \times 0.''36$	257	2018.1.01684.S	9.8	0.46
HNC	$2-1$	181.3248	13.1	$0.''34 \times 0.''30$	210	2018.1.00321.S	6.0	0.41

Notes. Molecular transitions observed as part of the ALMA projects 2018.1.01506.S, 2018.1.01684.S, and 2018.1.00321.S. Rest frequencies and upper-level energies are taken from the Cologne Database for Molecular Spectroscopy (CDMS; [Endres et al. 2016](#)). The column “Regions $> 3\sigma$ ” lists the number of hexagons where the integrated intensity exceeds a signal-to-noise ratio of three. The MRS corresponds to the largest angular scale recoverable by the observations. The RMS shows the channel noise level measured after convolving the cubes to a resolution of $0''.8$.

those regions that satisfy a specified signal-to-noise ratio threshold, in our case $S/N \geq 3$. The noise on the moment 0 map, σ_{mom0} (in Jy beam⁻¹ km s⁻¹), was calculated using the noise in one line-free channel, σ_{chan} (in Jy beam⁻¹); the number of channels included for each pixel in the moment 0 map, N_{chan} , and the velocity resolution, ΔV (in km s⁻¹): $\sigma_{\text{mom0}} = \sigma_{\text{chan}} \sqrt{N_{\text{chan}}} \Delta V$.

Although this approach leaves some hexagons with measurements for only a few species, it captures genuine spatial variations in molecular content across NGC 1068. We therefore analyzed only hexagonal regions with more than five detected transitions (see Section 3.4).

3. Bayesian and neural network workflow

To characterize the global molecular gas properties and to investigate whether the outflow launched from the AGN reaches the starburst ring, we developed a modeling framework that combines chemical evolution, radiative transfer, and Bayesian inference. The chemical abundances are computed with UCLCHEM ([Holdship et al. 2017](#))², a gas grain chemical modeling code that uses user-defined chemical networks and physical modules to simulate a wide range of conditions. In this work, we employ two types of chemical models: a quiescent cloud model and a heating model. The two models differ only in their temperature evolution, where the heating model allows the temperature to rise gradually to mimic the effect of stellar or AGN activities, while the quiescent model holds the temperature fixed. In the quiescent model, the gas temperature is held at the input value throughout the chemical evolution, whereas in the heating model the gas starts at 10 K and increases gradually to the specified final temperature. Because the chemical network is time-dependent, this difference in thermal history produces distinct molecular abundances even when both models reach the same final temperature. We performed radiative transfer calculations using SpectralRadex³ ([Holdship et al. 2021](#))⁴. This code, based on RADEX ([van der Tak et al. 2007](#)), predicts molecular line intensities based on collisional rate coefficients obtained from the LAMBDA database ([Schöier et al. 2005](#))⁵. We adopted linewidths of 150, 100, and 50 km s⁻¹ for the CN, stellar bar, and starburst ring, respectively ([Scourfield et al. 2020](#)).

² <https://github.com/uclchem/UCLCHEM>

³ Our analysis confirms that all transitions remain optically thin at the best-fit parameters in all regions, particularly for C₂H, which consists of hyperfine structures.

⁴ <https://spectralradex.readthedocs.io>

⁵ <https://home.strw.leidenuniv.nl/~moldata/>

Bayesian inference is carried out with Nautilus ([Lange 2023](#)), which combines neural-network accelerated transport, importance sampling, and ultrafast likelihood approximations. This accelerated sampling strategy enables efficient exploration of high-dimensional posteriors and provides robust constraints on the physical conditions across the galaxy with reduced computational cost.

However, performing full chemical network calculations within the Bayesian inference process would be computationally prohibitive for analyzing the entire galaxy. To overcome this limitation, we implemented a neural network that can efficiently emulate the chemical evolution calculations, following the methods of [de Mijolla et al. \(2019\)](#), replacing UCLCHEM in our analysis pipeline (see Fig. 1). The neural network architecture is described in Sect. 3.1, and the Bayesian inference methodology is detailed in Sect. 3.4.

3.1. Neural network architecture

We constructed a neural network using the TensorFlow package to emulate the chemical modeling calculations. The network takes four inputs, corresponding to the chemical model parameters: kinetic temperature (T_K), H₂ volume density (n), cosmic-ray ionization rate (ζ), and H₂ column density (N_{H_2}). The architecture includes four hidden layers with 2048 nodes each. The output layer returns the predicted molecular abundances for the species considered in this study.

During training, we use a mean-squared-error loss function to quantify the difference between the neural network predictions and the abundances from the training data. This loss is used to update the network weights and biases throughout each epoch, where an epoch corresponds to one full pass through the training set. A separate validation set, not used during training, is evaluated at the end of each epoch to monitor the model’s performance on unseen data.

To prevent overfitting, we implemented an early stopping criterion that halts training when the validation loss has not improved over 20 consecutive epochs. The model then reverts to using the weights from the epoch with the lowest validation loss. This approach ensures the model generalizes well to new parameter combinations rather than simply memorizing the training data.

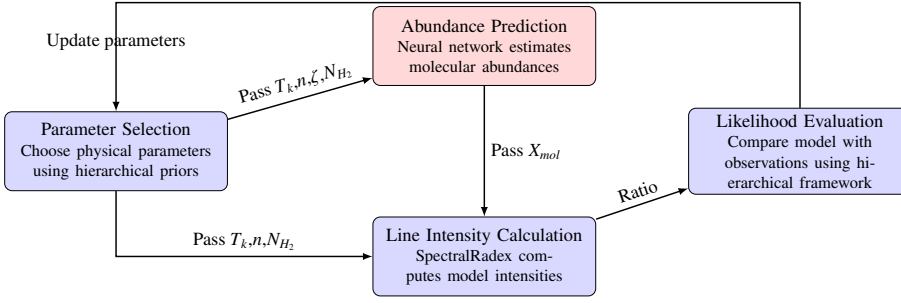


Fig. 1. Workflow of our hierarchical Bayesian analysis. The neural network component (red) accelerates the analysis by replacing computationally intensive chemical modeling. Each box shows a key step in the process, with arrows indicating the dataflow between steps. The feedback loop allows continuous refinement of parameter estimates until convergence is achieved.

3.2. Training dataset

Our neural network model was trained to predict molecular abundances using input parameters generated by UCLCHEM (see Table 2). UCLCHEM employs a two-stage modeling approach. In stage 1, a freefall collapse model simulates the conversion of atomic/ionic gas to molecular form under fixed physical conditions: initial density of 100 cm^{-3} , temperature of 10 K, with the standard cosmic ray ionization rate for molecular hydrogen of $\zeta_0 = 1.36 \times 10^{-17} \text{ s}^{-1}$ (e.g., Indriolo et al. 2015). This stage tracks chemical evolution over 6 Myr, with the final molecular abundances serving as initial conditions for stage 2. The second stage incorporates four of the parameters listed in Table 2 to model chemical evolution for an additional 1 Myr, by which time most reactions have reached chemical equilibrium. In this stage, we adopt a visual extinction of $A_V = 10$ mag for all models. At this extinction, the external UV radiation field is fully attenuated and UV driven photochemistry does not contribute to the chemical evolution (Scourfield et al. 2020; Holdship et al. 2021). This choice is supported by previous studies of NGC 1068, which infer molecular column densities throughout the CND and the starburst ring that imply visual extinctions well in excess of 10 mag (Scourfield et al. 2020; Butterworth et al. 2022). The column densities we derive (see Fig. 5) are consistent with this picture: adopting the conversion relation between N_{H_2} and A_V (Dyson & Williams 1980), all analyzed regions remain comfortably in the $A_V > 10$ mag regime. The final abundances from stage 2 constitute our neural network training dataset.

Table 2 presents the parameter ranges explored in our models, specifies the assumed prior distributions for each parameter, and indicates the number of sampled values within each range. This sampling scheme yielded 481,988 unique parameter combinations for our chemical modeling.

UCLCHEM solves coupled ordinary differential equations, and convergence problems can occur when the system is stiff. As noted by Heyl et al. (2023), such problems can produce unrealistically low molecular abundances that come from numerical error rather than real chemistry. To keep only physically meaningful results in our training set, we set a lower limit of 10^{-15} for fractional abundances and removed any outputs below this value. This choice is practical because abundances below 10^{-15} are far below our observational sensitivity.

We divided the UCLCHEM output into three subsets: a training set containing 80% of the data ($\sim 360,000$ points), a validation set with 10% ($\sim 40,000$ points), and a test set with the remaining 10% ($\sim 40,000$ points). The parameter values listed in Table 2 serve as inputs to the first layer of the neural network, which are then propagated through subsequent layers to generate molecular abundance predictions. Since our chemical abundances span eleven orders of magnitude (10^{-15} to 10^{-4}), normalization to $(-1, 1)$ prevents gradient vanishing for small values and centers

the data around zero, which improves the performance of ReLU activation functions and accelerates convergence.

Throughout each training epoch, we continuously monitor the mean-squared error loss between the network predictions and the actual training data. The validation loss, calculated using the validation dataset, is evaluated only after each epoch to assess the network’s generalization capability. Once the stopping criterion is met (see Sec. 3.1), we evaluate the trained model’s performance using the test set. We can quantitatively evaluate the model’s predictive accuracy by comparing the network’s abundance predictions for the test set against the corresponding UCLCHEM calculations.

3.3. Training results

Fig. 2 shows the performance of the neural network model using HNC as an example. The network reproduces the UCLCHEM predictions with a mean relative error of 0.35% and accurately recovers abundance variations spanning approximately eight orders of magnitude. A small number of outliers deviate from the true abundances by several orders of magnitude, and these cases occur mainly when the input volume density (n_{H_2}) or column density (N_{H_2}) lies close to the boundaries of the parameter space (Behrens et al. 2024). Although Behrens et al. (2024) introduced additional data points outside the target parameter ranges to mitigate this behavior, we do not extend the parameter space with buffer points because the current model performance is sufficient for our analysis and previous studies of NGC 1068 show that the molecular gas rarely reaches these boundary values (Viti et al. 2014; Scourfield et al. 2020; Huang et al. 2022; Butterworth et al. 2022). Similar performance results for other molecular species are shown in Fig. A.1.

3.4. Hierarchical Bayesian model

We infer the physical conditions of molecular gas using a hierarchical Bayesian (HB) framework following Tanaka et al. (2018) and Tanaka et al. (2024). The HB approach enables a self-consistent treatment of measurement uncertainties and additional non-statistical scatter, while constraining the population distribution of physical parameters across all regions.

For each region i , we define a parameter vector $\theta_i = (\log n_{\text{H}_2}, \log T_K, \log N_{\text{H}_2}, \log \zeta)_i$. These parameters describe the local physical state inferred from our non-LTE radiative transfer coupled with chemistry modeling. The ensemble of θ_i is modeled with a multivariate Student- t distribution with location parameter μ and covariance matrix Σ , which describes the intrinsic dispersion and correlations of the physical parameters across all regions.

In contrast to previous intensity-based implementations, we use line ratios as observables. For region i , the observed data vector is defined as $\mathbf{y}_i^{\text{obs}} = \ln(\mathbf{r}_i)$, where $\mathbf{r}_i$ contains ratios con-

Table 2: Prior distributions and training data.

Parameter	Description	Range	Distribution type	No. points
T_K^a	Temperature (K)	30-300	Log	26
n_{H_2}	Volume density (cm^{-3})	10^3 – 10^7	Log	23
ζ	Cosmic-ray ionization rate (ζ_0) ^b	1 – 10^3	Log	31
N_{H_2}	H_2 column density (cm^{-2})	10^{22} – 10^{25}	Log	26

Notes. ^(a) Maximum temperature in the heating model.

^(b) $\zeta_0 = 1.36 \times 10^{-17} \text{ s}^{-1}$

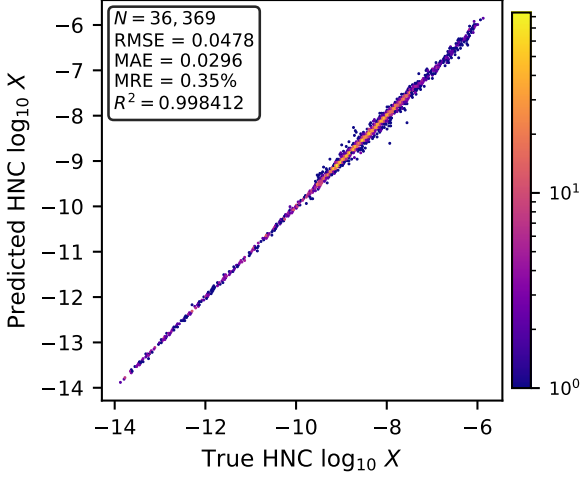


Fig. 2: Comparison between the HNC fractional abundances predicted by the neural network emulator and those computed by UCLCHEM for the test dataset containing 36,369 chemical models. The emulator accurately reproduces the chemical model predictions over approximately eight orders of magnitude in abundance (10^{-10} to 10^{-6}). The performance metrics show a root mean square error of 4.78×10^{-2} dex, a mean absolute error of 2.96×10^{-2} dex, and a mean relative error of 0.35%, with $R^2 = 0.9984$. These results demonstrate that the neural network provides a reliable surrogate for the chemical model across the explored parameter space.

structed from all available transitions with positive detections. To avoid over-weighting specific transitions, we construct $m = n - 1$ ratios in a chain form, where n is the number of transitions detected above 3σ in a given region. These ratios take the form $r_k = I_k/I_{k+1}$ for $k = 1, \dots, n - 1$, after sorting the transitions. Because adjacent ratios share common intensities, the elements of $\mathbf{y}_i^{\text{obs}}$ are correlated. We therefore adopt a multivariate normal likelihood: $\mathbf{y}_i^{\text{obs}} \sim \mathcal{N}(\mathbf{y}_i^{\text{mod}}, \mathbf{C}_i)$, where $\mathbf{y}_i^{\text{mod}}$ is the model prediction and $\mathbf{C}_i$ is the covariance matrix derived from measurement uncertainties and ratio propagation.

To account for residual non-statistical effects such as calibration systematics and modeling imperfections, we introduce an additive term in log-ratio space: $\mathbf{y}_i^{\text{obs}} = \mathbf{y}_i^{\text{mod}} + \boldsymbol{\epsilon}_i$, where $\boldsymbol{\epsilon}_i$ follows a normal distribution with zero mean and global scale parameter σ_{error} . This corresponds to a multiplicative factor in ratio space, consistent with the formulation in Tanaka et al. (2024).

The population covariance matrix is decomposed as $\boldsymbol{\Sigma} = \mathbf{S}\mathbf{R}\mathbf{S}$, where $\mathbf{S}$ is a diagonal matrix that sets the scale of each parameter, and $\mathbf{R}$ is the correlation matrix. This decomposition separates the marginal dispersions from the parameter correla-

Table 3: Hyperparameters and prior ranges adopted in the hierarchical Bayesian analysis.

Parameter	Prior range
Location parameters ($\boldsymbol{\mu}$)	
μ_n	(3.0, 6.00)
μ_T	(1.55, 2.30)
μ_N	(22.5, 24.0)
μ_ζ	(0.0, 2.0)
Scale parameters ($\mathbf{S}$)	
σ_n	(0.1, 1.0)
σ_T	(0.1, 0.8)
σ_N	(0.1, 1.0)
σ_ζ	(0.1, 0.5)
Correlation coefficients ($\mathbf{R}$)	
R_{nT}	(0.0, ...)
R_{nN}	(0.0, ...)
$R_{T\zeta}$	(0.0, ...)
$R_{N\zeta}$	(..., 0.0)
Non-statistical scatter	
σ_{error}	(0.02, 0.5)

Notes. All physical parameters are defined in logarithmic scale. The population covariance matrix is written as $\boldsymbol{\Sigma} = \mathbf{S}\mathbf{R}\mathbf{S}$. The correlation matrix $\mathbf{R}$ is constructed to be positive definite, and the listed ranges are implemented as soft bounds.

tions and improves numerical stability during sampling. The correlation matrix is parameterized through a lower-triangular form to guarantee positive definiteness. We impose soft constraints on selected correlation coefficients in order to suppress unphysical degeneracies between strongly coupled parameters. In particular, we allow positive correlations between N_{H_2} and n_{H_2} , and between T_K and ζ , while a negative correlation is favored between N_{H_2} and ζ , consistent with Padovani et al. (2018). Although the correlation between n_{H_2} and T_K is not immediately intuitive, it has been reported for the Galactic center (Nagai et al. 2007; Tanaka et al. 2018) and in extragalactic hierarchical Bayesian studies (Tanaka et al. 2024). We note, however, that in our analysis the final posterior distributions do not show a significant change whether this correlation is imposed or not. The adopted hyperparameters and their prior ranges are summarized in Table 3.

Under this hierarchical structure, the joint posterior distribution is written as

$$P(\boldsymbol{\Theta}, \boldsymbol{\epsilon}, \boldsymbol{\eta} \mid \mathbf{Y}) \propto P(\mathbf{Y} \mid \boldsymbol{\Theta}, \boldsymbol{\epsilon}) P(\boldsymbol{\Theta}, \boldsymbol{\epsilon} \mid \boldsymbol{\eta}) P(\boldsymbol{\eta}). \quad (1)$$

Here $\mathbf{Y} = \{\mathbf{y}_i^{\text{obs}}\}$ is the set of observed log-ratio vectors, $\boldsymbol{\Theta} = \{\boldsymbol{\theta}_i\}$ are the region parameters, $\boldsymbol{\epsilon} = \{\boldsymbol{\epsilon}_i\}$ are the non-statistical error terms, and $\boldsymbol{\eta} = \{\boldsymbol{\mu}, \boldsymbol{\Sigma}, \sigma_{\text{error}}\}$ denotes the hyperparameters. The HB inference yields posterior probability distributions of T_K , n_{H_2} , N_{H_2} , and ζ for each 56 pc region, together with 68% credible intervals.

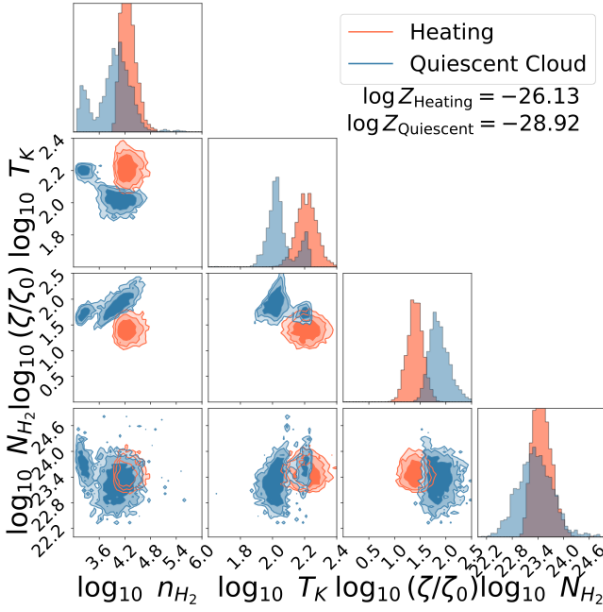


Fig. 3: Corner plots showing the Bayesian inference results for a molecular cloud near the CND-S. Orange and blue colors correspond to the heating and quiescent cloud models. Contours show the 50, 80, and 95 percent credible intervals. The log-evidence values indicate that the heating model is preferred.

4. Results

In this section, we present the results of our hierarchical Bayesian analysis of the molecular gas in NGC 1068. The framework yields posterior constraints on the physical conditions of the gas, including density, temperature, cosmic-ray ionization rate (CRIR), and column density. These parameters enable us to construct detailed physical parameter maps across NGC 1068, revealing spatial gradients that trace the signatures of AGN-driven outflow through the galaxy.

4.1. Posterior results and model preference

We identified 198 regions where more than five molecular transitions are detected above the three-sigma level, ensuring that the number of observational constraints exceeds the number of free parameters in the Bayesian inference. Figure 3 presents an example of the posterior distributions for one of the subregions listed in Table 4, located near the CND-S. The posteriors are shown for both the heating and quiescent cloud models. The Bayesian evidence ($\log Z$) provides an objective criterion for model selection, as it measures the marginal likelihood averaged over the full parameter space. A higher value indicates stronger support when both fit quality and model complexity are taken into account. In this representative region, the evidence values are -26.13 for the heating model and -28.92 for the quiescent model. The difference of 2.8 in log-evidence corresponds to a Bayes factor of $\exp(2.8) \approx 16$, which provides strong support for the heating model.

We then construct a spatial model-selection map using the difference in Bayesian evidence (Fig. 4). Regions of particular interest are marked with different symbols. Circles denote subregions in the CND and the AGN, squares indicate super-star clusters (SSCs) in the starburst ring, and a pentagram marks the position of Type II SN 2018ivc (Bostroem et al. 2020). The SSC positions are adopted from Rico-Villas et al. (2021), where

Table 4: Subregion coordinates in NGC 1068.

Subregion	RA (J2000)	Dec (J2000)
E Knot	02 ^h 42 ^m 40.771 ^s	−00°00′47.84″
W Knot	02 ^h 42 ^m 40.630 ^s	−00°00′47.84″
AGN	02 ^h 42 ^m 40.710 ^s	−00°00′47.94″
CND-N	02 ^h 42 ^m 40.710 ^s	−00°00′47.09″
CND-S	02 ^h 42 ^m 40.710 ^s	−00°00′49.87″
SHC	02 ^h 42 ^m 40.84 ^s	−00°00′32.94″
SSC 1	02 ^h 42 ^m 41.44 ^s	−00°00′37.48″
SSC 2	02 ^h 42 ^m 41.29 ^s	−00°00′34.97″
SSC 3	02 ^h 42 ^m 41.15 ^s	−00°00′34.64″
SSC 4	02 ^h 42 ^m 40.32 ^s	−00°00′32.66″
SSC 5	02 ^h 42 ^m 40.12 ^s	−00°00′35.87″
SSC 6	02 ^h 42 ^m 39.95 ^s	−00°00′37.75″
SSC 7	02 ^h 42 ^m 39.84 ^s	−00°00′53.12″
SSC 8	02 ^h 42 ^m 39.88 ^s	−00°00′54.96″
SSC 9	02 ^h 42 ^m 39.95 ^s	−00°00′57.88″
SSC 10	02 ^h 42 ^m 40.13 ^s	−00°01′00.76″
SSC 11	02 ^h 42 ^m 40.30 ^s	−00°01′01.64″
SSC 12	02 ^h 42 ^m 40.44 ^s	−00°01′02.85″
SSC 13	02 ^h 42 ^m 40.59 ^s	−00°01′01.61″
SSC 14	02 ^h 42 ^m 40.65 ^s	−00°01′00.95″
SN2018ivc	02 ^h 42 ^m 41.29 ^s	−00°00′31.71″

$\text{Pa}\alpha$ emission was used to trace compact young stellar clusters. The coordinates of all marked subregions are provided in Table 4. Regions within the CND along the AGN wind direction show the strongest preference for the heating model, consistent with previous studies that identified outflow-driven disturbances in these areas (García-Burillo et al. 2014, 2019). Some regions outside the ionized bicone also favor heating, in agreement with non-rotational CO(2–1) motions extending beyond the bicone (García-Burillo et al. 2014; Zhang et al. 2025). In contrast, regions located further from the AGN, on the eastern side of the East Knot and the western side of the West Knot, preferentially support the quiescent model, consistent with the absence of clear outflow signatures in those areas.

Several regions along the jet direction on the eastern side correspond to the arc features seen by García-Burillo et al. (2014). High-sensitivity *e*-MERLIN and VLA images from Mutie et al. (2024) show that the NE arc has a spectral index of -1.1 ± 0.1 , typical of optically thin synchrotron emission, indicating strong jet–ISM interaction. These regions also favor the heating model, supporting this interpretation. A shock model would likely better describe these conditions, but since shock-based emulators are still in development, we focus here on the heating–quiescent comparison.

In the northern starburst ring, regions near the SSCs, compact young stellar clusters associated with intense star formation, and at the bar–ring interface favor the heating model, consistent with strong cloud compression. The average log-evidence difference exceeds 3. The northwestern starburst ring, however, shows mixed behavior: areas outside the SSCs favor the quiescent model, suggesting that molecular clouds at ~ 50 pc resolution remain largely unperturbed. The southern starburst ring shows a layered pattern. The bar–ring interface again favors heating, while regions slightly farther out lean toward the quiescent model, implying weaker external influence. At the outer edge, the heating model dominates once more. Rico-Villas et al. (2021) showed that gas responds to the spiral inside corotation by entering the spiral arm, where accumulation and/or compression triggers star formation. Our results align with this picture,

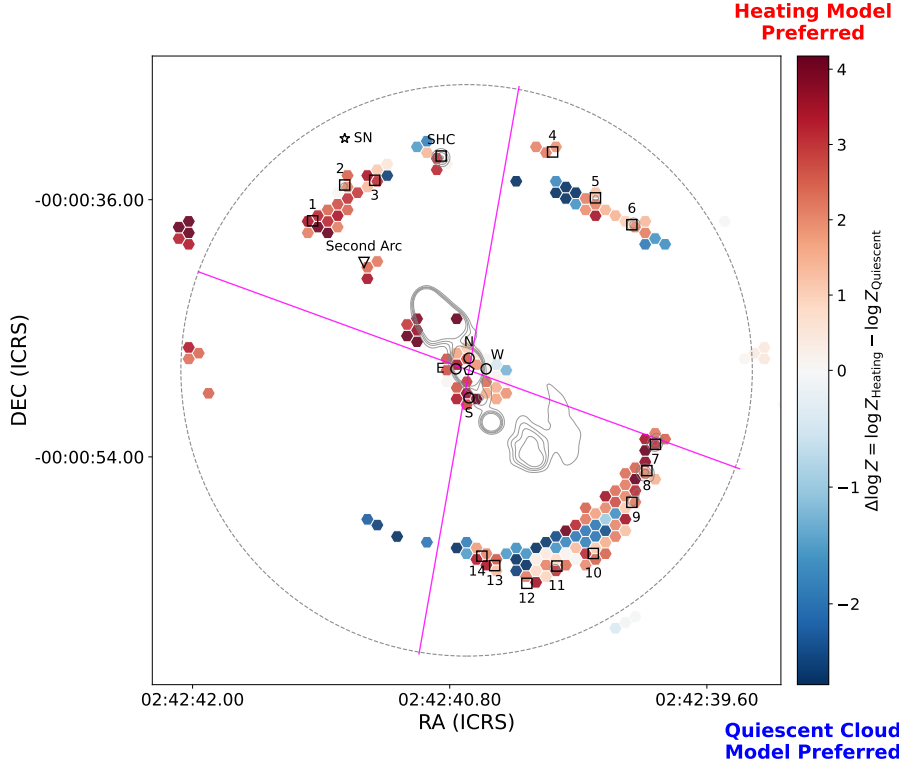


Fig. 4. Spatial distribution of the difference in log-evidence between the heating and quiescent models across the CND and the starburst ring. Red colors indicate support for the heating model, and blue colors indicate support for the quiescent model. Contours show the 100 GHz continuum map, and symbols mark regions of interest. Labels denote the corresponding SSCs and subregions in the CND. The magenta line outlines the region possibly influenced by the AGN wind described by Das et al. (2007).

as the outer starburst ring edge appears to host gas undergoing active heating and star formation.

4.2. Physical properties of the cloud

Fig. 5 presents the physical parameters derived from the HB model. We analyzed the parameter statistics across the three main regions of NGC 1068 (CND, stellar bar, and starburst ring), revealing distinct physical conditions in each environment. The CND exhibits the highest molecular gas density ($n_{\text{H}_2} \approx 10^{4.42 \pm 0.31} \text{ cm}^{-3}$), denser than the starburst ring ($n_{\text{H}_2} \approx 10^{4.17 \pm 0.32} \text{ cm}^{-3}$) and the stellar bar ($n_{\text{H}_2} \approx 10^{3.78 \pm 0.29} \text{ cm}^{-3}$). This trend is consistent with previous studies (Viti et al. 2014; Scourfield et al. 2020; Butterworth et al. 2022), although we note that the exact values might not match those from previous studies, and such differences are discussed in Section 5.1. Similar trends are observed in the H_2 column density, with the CND showing the highest values ($N_{\text{H}_2} \approx 10^{23.52 \pm 0.34} \text{ cm}^{-2}$), followed by the starburst ring ($N_{\text{H}_2} \approx 10^{23.23 \pm 0.33} \text{ cm}^{-2}$) and the stellar bar ($N_{\text{H}_2} \approx 10^{22.84 \pm 0.31} \text{ cm}^{-2}$).

The kinetic temperature distribution reveals that the stellar bar exhibits the highest mean temperature ($T_{\text{kin}} = 140.8 \pm 36.6 \text{ K}$), substantially exceeding both the CND ($T_{\text{kin}} = 82.2 \pm 28.3 \text{ K}$) and the starburst ring ($T_{\text{kin}} = 76.2 \pm 28.1 \text{ K}$). This temperature enhancement in the stellar bar is consistent with expectations for regions proximate to the jet (Mutie et al. 2024), where mechanical heating and cosmic ray heating contribute to elevated temperatures. The southern starburst ring displays higher temperatures than its northern counterpart, which may be attributed to the presence of younger SSCs (Rico-Villas et al. 2021). A similar temperature gradient linked to SSC evolution has been observed in NGC 4945: Bellocchi et al. (2023) found that the youngest proto-SSCs have rotational temperatures of about 65 K, much higher than the 25 K measured in more evolved SSCs. In early stages, strong protostellar activity and feedback heat the

surrounding molecular gas. As SSCs evolve, heating becomes confined to H II regions while the larger molecular cloud cools, producing the observed decline in temperature.

The CRIR remains uniformly high across the central kiloparsec, with only a moderate decline toward the outer regions. The CND shows the highest mean value, $\log(\zeta/\zeta_0) \approx 1.95 \pm 0.21$, followed by the stellar bar (1.91 ± 0.23) and the SSCs in the starburst ring (1.88 ± 0.24). The molecular clouds not associated with SSCs show a more pronounced decrease, with an average of 1.03 ± 0.21 . The elevated CRIR in the CND likely originates from particle acceleration near the AGN or within AGN-driven outflows (e.g., Rodrigues et al. 2021). The similar values found in the bar suggest that jet–ISM interactions or large-scale shocks maintain a high level of cosmic ray activity there, consistent with observations of cosmic ray production in jet systems such as Centaurus A (H. E. S. S. Collaboration et al. 2020). The slightly lower but still enhanced CRIR in the starburst ring is consistent with cosmic ray generation by clustered supernovae and massive stellar winds in active star-forming regions (Holdship et al. 2022; Behrens et al. 2024). The overall distribution therefore points to a broadly elevated cosmic ray field across the CND, bar, and SSCs, with a clear reduction only in the more quiescent molecular clouds.

5. Discussion

In this section, we first compare our results with previous work to establish consistency with earlier studies of NGC 1068. We then investigate whether the AGN-driven outflow affects the starburst ring by analyzing physical parameter gradients along the outflow trajectory and across the ring, with particular focus on regions at the inner edges of the northern and southern starburst rings. Finally, we present a preliminary analysis of CO(1–0) line profiles, demonstrating that single-Gaussian fits inadequately de-

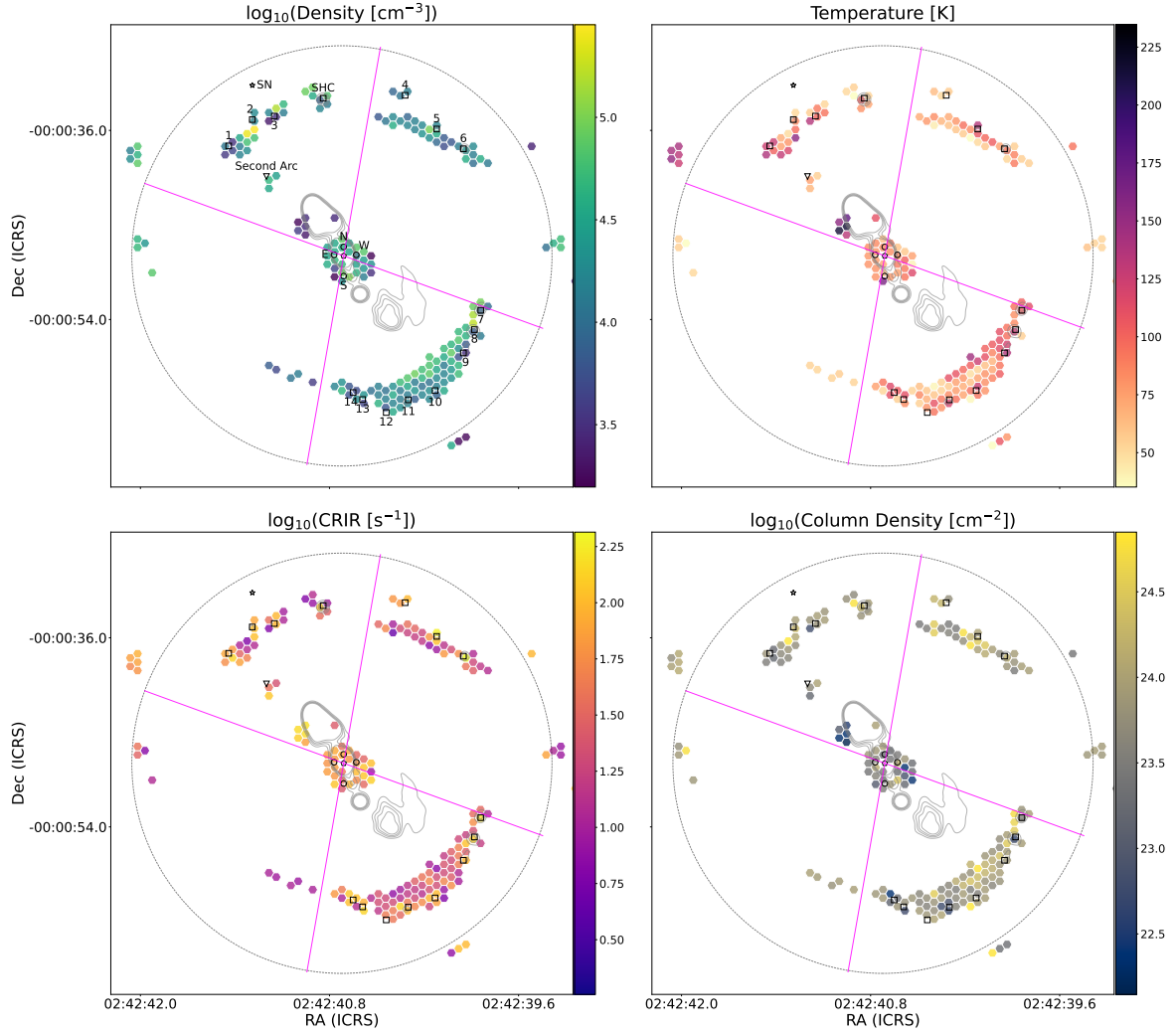


Fig. 5: Physical parameters derived in NGC 1068. The panels show the spatial distribution of molecular gas properties: volume density (upper left), kinetic temperature (upper right), cosmic ray ionization rate (lower left), and column density (lower right). Labels denote the corresponding SSCs and subregions in the CND, and are listed in the density panel.

scribe the emission in the starburst rings, which provides additional evidence of outflow activity.

5.1. Comparisons with previous studies

We compared our results with previous multi-molecular studies of NGC 1068 in Fig. 6, focusing on [Butterworth et al. \(2022\)](#), [Viti et al. \(2014\)](#), and [Scourfield et al. \(2020\)](#). For [Viti et al. \(2014\)](#) and [Scourfield et al. \(2020\)](#), we adopt the parameters derived from their best fit UCLCHEM models to remain consistent with the coupled chemical and radiative transfer framework used in this work. Although [Butterworth et al. \(2022\)](#) did not include chemical modeling, the overlap in molecular tracers makes their results suitable for comparison. More details of those previous studies are summarized in Appendix E.

The largest discrepancies among studies are found in the derived gas densities within the CND, particularly in the E-knot and W-knot, where our values are systematically lower than those reported previously. This difference likely reflects a combination of spatial sampling and tracer selection. These regions may not be fully sampled by our hexagonal grid, and the area-weighted averaging of overlapping hexagons may incorporate

lower density surroundings. More importantly, our analysis relies on low-J transitions, which are less sensitive to dense gas than the high-J transitions used in earlier work, consistent with [Butterworth et al. \(2022\)](#), who showed that low-J HCN is not an effective tracer of high-density material. Due to the limited number of available molecular constraints in the innermost CND, likely related to the strong ionized outflow ([García-Burillo et al. 2014](#); [Huang et al. 2022](#); [Vollmer et al. 2022](#)), we do not derive physical parameters for the AGN region. In the CND-N and CND-S regions, our density estimates agree more closely with [Butterworth et al. \(2022\)](#), while the larger offsets relative to [Viti et al. \(2014\)](#) and [Scourfield et al. \(2020\)](#) can be attributed to differences in chemical model sampling, since their parameter grids were limited in size and unlikely to capture the strong chemical differentiation across the CND.

In the starburst ring, discrepancies in densities are mainly confined to NSB-a and SSB-a. These regions host very young SSCs with ages of order 10^5 years ([Rico-Villas et al. 2021](#)), and previous studies have shown that clusters at this stage can disperse nearby gas (e.g., [Miura et al. 2018](#); [Mills et al. 2021](#); [Sun et al. 2024](#)). The differences we find likely arise because our ~ 50 pc resolution beam contains multiple gas components. Young SSCs create low-density environments in their immedi-

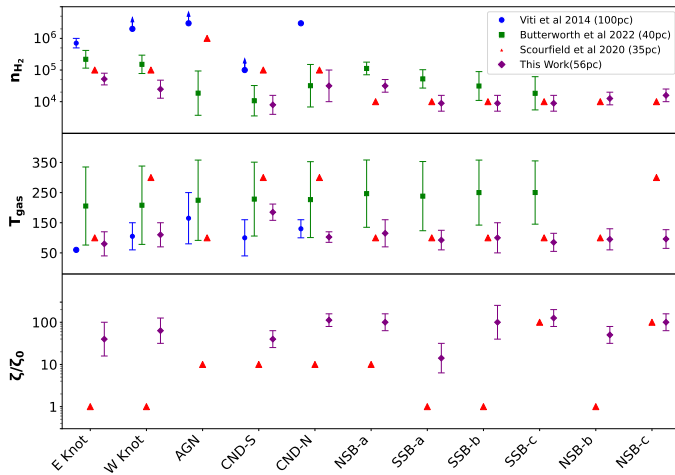


Fig. 6: Comparison of H_2 volume density, kinetic temperature, and cosmic ray ionization rate across different regions in NGC 1068. Values are shown for the E-knot, W-knot, CND-N, CND-S, and selected starburst ring regions. Results from Viti et al. (2014) at 100 pc resolution, Butterworth et al. (2022) at 40 pc resolution, Scourfield et al. (2020) at 35 pc resolution, and this work at 56 pc resolution are shown for reference.

ate surroundings, yet dense clumps can still exist within the beam. Different molecules therefore trace different phases that cannot be separated at this scale. This naturally leads to lower inferred densities compared to studies that rely on higher excitation transitions, such as Butterworth et al. (2022), and indicates that different datasets probe different components of the interstellar medium rather than inconsistent physical conditions.

For kinetic temperature (the second row in Fig. 6), the main discrepancies arise when comparing our results with Scourfield et al. (2020). In particular, our temperature estimates for the W-knot, CND-N, and CND-S are higher than those reported in their study. This difference likely reflects their reliance on CS transitions alone and the use of a sparse temperature grid, limited to 100 and 300 K, which restricts the ability to capture the full range of conditions present within the CND. In contrast, the temperature we derive within the CND is broadly consistent with Viti et al. (2014), although their lower spatial resolution of about 100 pc smooths over the temperature variations that we resolve, naturally leading their estimates toward lower values.

The cosmic ray ionization rate (the third row in Fig. 6) shows large variation among studies, particularly when compared with the CS-based analysis of Scourfield et al. (2020). This difference reflects the limitation of using a single molecular species to trace ionization level. Although our results disagree with Scourfield et al. (2020) for several subregions, both studies indicate that the ionization rate in these regions remains below about $100 \zeta_0$, a regime where the CS abundance becomes strongly non-linear (see Fig. C.1). This behavior makes the CRIR derived from CS alone unreliable compared with our multi-species approach.

5.2. The outflow impact

In this section, we examine whether the AGN-driven outflow in NGC 1068 influences star formation activity within the starburst ring. To address this question, we analyze the spatial distribution of physical parameters (Sec. 5.2.1), search for signatures of gas

compression caused by the outflow and investigate CO(1–0) line profiles across the galaxy (Sec. 5.2.2).

5.2.1. Gas density enhancement

In Fig. 5, we presented the physical parameters throughout the galaxy. Given that the aim of this work is to investigate the impact of the outflow on the starburst ring, we focus our analysis on regions beyond the CND. The arc regions (see Fig. 7) show clear signatures of jet influence, exhibiting relatively low densities ($\sim 10^3 \text{ cm}^{-3}$). Such reduced densities are consistent with strong jet–ISM interaction scenario, which can disturb or partially remove molecular gas through enhanced turbulence and cloud disruption, as shown in numerical simulations (Laužikas & Zubovas 2024) and in observational studies (e.g., Quillen et al. 2005; Arce et al. 2010). The arc regions also exhibit the highest gas temperatures measured in our study, indicating the extreme physical conditions present.

Moving outward from the CND toward the starburst ring along the jet propagation direction reveals distinct patterns in the gas properties. The second arc regions (Green triangle in Fig. 5), situated between the starburst ring and the primary arc structures, display significantly enhanced gas densities ($\sim 10^5 \text{ cm}^{-3}$) and lower gas temperatures ($\sim 60 \text{ K}$). These physical properties, together with the characteristic V-shaped morphology traced by the CO emission (Fig. 7), suggest that although the region is not directly impacted by the jet, compression associated with jet-driven outflows likely contributes to the observed molecular gas structure and influences the local physical conditions.

The northeastern starburst ring shows spatial variations in gas density that point to two different feedback effects. In regions that coincide with the SSCs, the gas density is systematically lower than in the surrounding regions, consistent with the removal or dispersal of gas by stellar winds from the young clusters (e.g., Pabst et al. 2019; Rosen 2022; Bonne et al. 2022). In contrast, nearby regions that do not overlap with any SSC exhibit density enhancements above 10^4 cm^{-3} . When these values are compared with the northwestern ring, where densities remain below 10^4 cm^{-3} , the enhanced densities are consistent with a scenario in which the outflow compresses the gas in these locations, although other mechanisms such as cloud collisions cannot be excluded. The observed pattern therefore suggests that stellar winds reduce the gas content around the SSCs, while the outflow may contribute to gas compression in adjacent clouds.

The southwestern starburst ring displays less fragmentation than its northern counterpart. Similar density patterns emerge near the bar-ring interface region, where decreased densities within SSCs are accompanied by elevated densities in surrounding molecular material. Sánchez-García et al. (2022) attributed the significant compression of molecular gas at the bar-ring interface to intense cloud-cloud collisions. In their analysis, the degree of gravitational boundedness of the dense gas was quantified through the parameter $b \equiv \Sigma_{\text{dense}}/\sigma^2$, which is proportional to the inverse of the virial parameter and measures the balance between self-gravity and kinetic energy of the gas, following the methodology of Leroy et al. (2017). A higher value of b indicates gas that is more gravitationally bound and therefore more likely to form stars efficiently. Our results are consistent with this scenario; however, we note that the boundedness parameter method has important limitations. As demonstrated in their study, the boundedness parameter shows significant scatter at the native resolution of $\sim 56 \text{ pc}$, with correlations only becoming statistically significant when averaged over larger scales ($\geq 100 \text{ pc}$). Furthermore, the parameter assumes virial equilibrium, which

may not hold in regions experiencing strong dynamical perturbations from outflows or cloud-cloud collisions. Additionally, we identify density enhancements exceeding 10^4 cm^{-3} accompanied by elevated temperatures ($>120 \text{ K}$) at the inner edge of the southwestern starburst ring. The spatial coincidence of enhanced density and temperature in this region, combined with its location relative to the outflow axis, suggests that outflow-driven compression rather than cloud-cloud collisions may be the dominant mechanism in this particular zone.

We note that while the combined density and temperature measurements provide valuable insights into the physical conditions across the starburst ring, these diagnostics alone cannot definitively distinguish between the various compression mechanisms at play. The observed enhancements are consistent with both jet-driven compression through ram pressure (e.g., [Wagner et al. 2012](#)) and shock compression from cloud-cloud collisions at the bar-ring interface (e.g., [Choi et al. 2023](#); [Maity et al. 2024](#); [Maeda et al. 2025](#)), as moderate-strength shocks from different physical origins produce similar signatures in our observed parameter range. Furthermore, projection effects and beam averaging may blend regions experiencing different mechanisms, particularly where the outflow influence zone overlaps with the bar-ring interface. Detailed kinematic analysis, which can reveal shock velocities and systematic velocity patterns associated with different acceleration mechanisms, will be required to disentangle these possibilities and will be addressed in future work. For the present analysis, we proceed with the understanding that significant compression is occurring throughout the starburst ring, with the specific driving mechanisms likely varying spatially depending on proximity to the jet axis and the bar-ring interface.

5.2.2. CO line profiles

In the previous sections, we investigated the potential effects of the outflow on the molecular gas properties. Here, we examine more direct evidence of gas outflow motion through analysis of CO line profiles. While detailed line profile analysis and kinematic modeling are beyond the scope of this work, we present a preliminary examination of outflow signatures in the CO line profiles across the galaxy.

Within the CND, we present CO line profiles from the E-knot and W-knot (middle-bottom subplots in Fig. 7). Single-component Gaussian fits clearly fail to reproduce the observed profiles. Indeed, [Zhang et al. \(2025\)](#) performed comprehensive line profile fitting in the CND regions and concluded that the E/W-knot require at least two velocity components to adequately fit the CO line profiles, providing evidence of molecular outflow.

The arc and second arc regions (second column, third and fourth rows in Fig. 7) exhibit pronounced absorption features at both blue- and red-shifted velocities. While missing flux may contribute to these features, the single-component fit to the main emission is insufficient, and additional components with different central velocities would be required to adequately reproduce the observed profiles, which may indicate the presence of multiple kinematic components along the line of sight.

We examine three CO(1–0) line profiles extracted from the inner edge of the northern SB ring (regions N-SB-Bar, N-SB-Bar-2, and N-SB-Bar-3; see the second column of the second row, the first row, and the first column of the first row in Fig. 7) and compare them with three spectra at nearby SSC positions (SSC1, SSC2, and SSC3). The SSC spectra are well described by single, nearly symmetric Gaussian components with FWHM values of 55.74 , 51.94 , and 46.59 km s^{-1} , while

the N-SB-Bar spectra, although not systematically broader in FWHM (one is comparable at 55.85 km s^{-1} and the other two are narrower at 37.88 and 40.00 km s^{-1}), are markedly more non-Gaussian: all three exhibit extended blue wings reaching $v \lesssim -150 \text{ km s}^{-1}$ and redward depressions/absorption-like dips around $+20$ to $+120 \text{ km s}^{-1}$, and in some cases an additional blue component is present. We present the spectra extracted from the N-SB-Bar-2 region, where both the CO(1–0) and $^{13}\text{CO}(1–0)$ profiles display clear signatures of complex kinematics, as shown in Fig. 8. The appearance of a secondary peak at -120 km s^{-1} in both transitions confirms this feature is intrinsic to the gas rather than an artifact of CO self absorption, while the extended blue wing in the CO emission suggests the presence of outflowing molecular gas across this region.

At the inner edge of the southern starburst ring, we examine three regions, S-SB-IE-1, S-SB-IE-2, and S-SB-IE-3 (fifth column third row, sixth column third row, and fifth column fourth row in Fig. 7, respectively). The CO spectra reveal diverse kinematic structures. S-SB-IE-1 shows extended wing-like emission on both the redshifted and blueshifted sides of the main component, suggesting the presence of dynamically disturbed gas, potentially associated with outflowing motions. S-SB-IE-2 exhibits a more localized excess near $+200 \text{ km s}^{-1}$, with a stronger high-velocity contribution than in the surrounding regions. S-SB-IE-3 presents a pronounced double-peaked structure centered near $+100 \text{ km s}^{-1}$. We also inspected the corresponding $^{13}\text{CO}(1–0)$ spectra to assess the robustness of these features. However, none of the regions displays a clear counterpart to the excess emission near $+200 \text{ km s}^{-1}$, and in particular the secondary contribution seen in CO in S-SB-IE-2 is not detected in ^{13}CO . For S-SB-IE-3, the limited velocity resolution and modest signal-to-noise prevent us from confirming the presence of the weak feature near $+150 \text{ km s}^{-1}$. Taken together, these profiles likely trace a mixture of kinematic components, and their morphology may reflect CO self-absorption (e.g., [Combes et al. 2019](#); [Rose et al. 2019, 2020](#)) or the superposition of multiple gas structures along the line of sight.

While determining the precise origin of these complex CO line profiles is beyond the scope of this work, the comparison between regions along the proposed outflow trajectory and those in the starburst rings provides suggestive evidence of outflow activity. The observed absorption features at the line wings and the double-peaked profiles warrant detailed investigation in future work.

6. Conclusions

We have combined high resolution ALMA observations with a hierarchical Bayesian framework that links non-LTE radiative transfer and chemical modeling to study the molecular gas in NGC 1068. By using a trained neural network emulator, we achieved efficient inference without losing predictive accuracy. This approach allowed us to derive spatially resolved distributions of gas density, temperature, column density, and cosmic-ray ionization rate across both the CND and the starburst ring. Our main findings can be summarized as follows:

1. The inferred physical parameters show clear radial and azimuthal variations. The CND displays higher temperatures and ionization rates than the starburst ring, while the ring hosts cooler and denser gas associated with star formation.
2. Enhanced gas density and elevated temperatures are found along the inner edge of the starburst ring, suggesting that the nuclear outflow influences the local gas conditions beyond the CND.

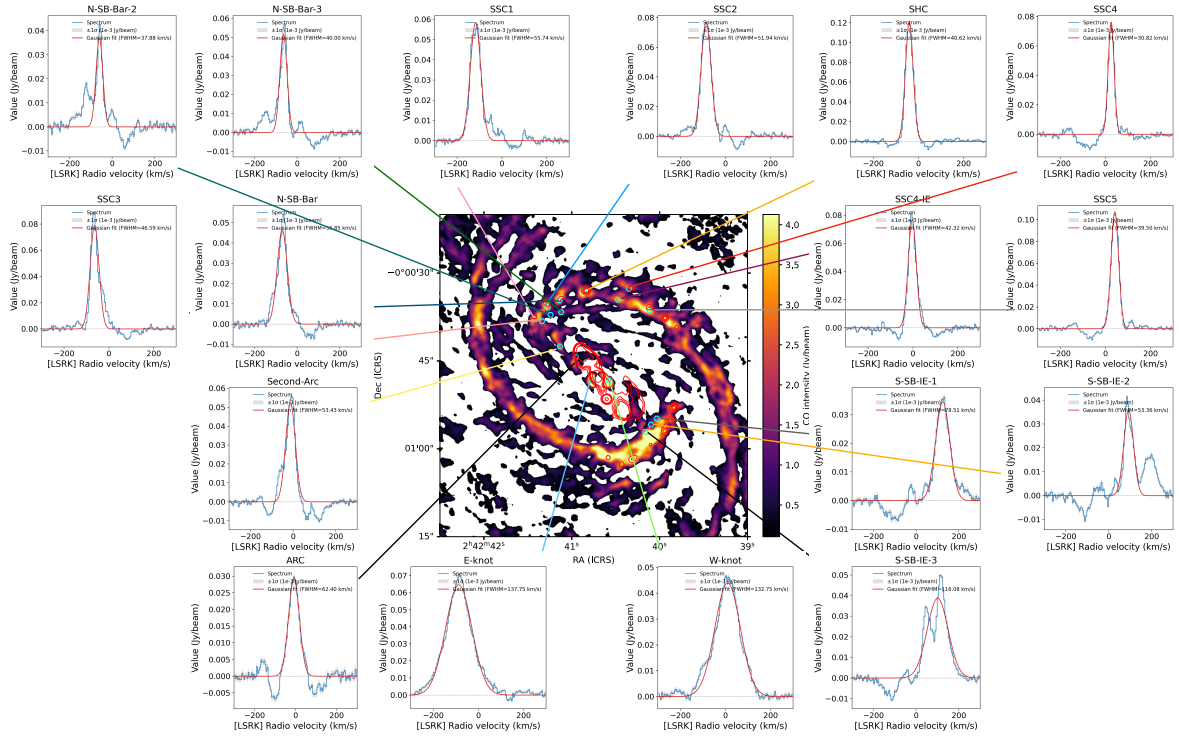


Fig. 7: CO(1–0) line profiles across NGC 1068. The color map shows the CO(1–0) integrated intensity, with red contours representing the 100 GHz continuum emission at 5σ , 10σ , 15σ , 20σ , and 100σ levels. Line profiles were extracted from hexagonal apertures of identical size. Each panel shows the observed spectrum (blue), the 1σ noise level (gray), and a single-component Gaussian fit (red) to the emission above zero intensity. The hexagon positions and extraction regions are indicated on the map.

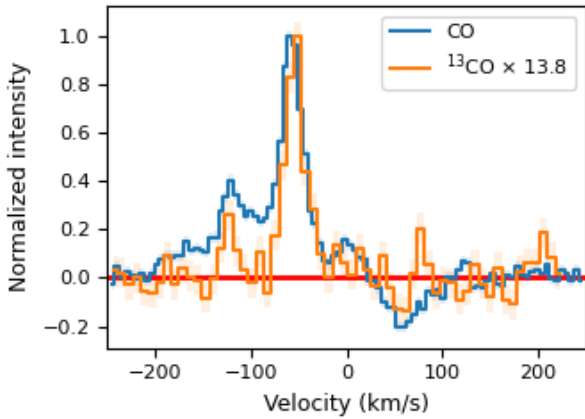


Fig. 8: CO(1–0) (blue) and $^{13}\text{CO}(1-0)$ (scaled by a factor of 13.8, orange) line profiles extracted from the inner edge of the NE starburst ring. The secondary peak located at -120 km s^{-1} appears in both transitions. The error bars indicate the rms noise per velocity channel measured from line-free regions of the spectrum.

- Line profiles of CO (1–0) exhibit non-Gaussian features in regions near the outflow path, consistent with the presence of disturbed kinematics or multiple gas components.
- Comparison with previous single-pointing studies shows broad consistency, but our spatially resolved modeling highlights sub-structure that could not be captured by earlier analyses.

These results demonstrate the capability of combining chemistry and radiative transfer calculation to interpret molecular

emission on galactic scales. The method provides a practical way to investigate how feedback from an active nucleus reshapes the surrounding interstellar medium. Future extensions that include higher resolution observation, shock tracers, and time-dependent emulator will help better disentangle heating, turbulence, and chemical effects in NGC 1068 and other nearby active galaxies.

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Appendix A: Neural network performance

Figure A.1 summarizes the performance of the trained neural network for all species used in this work. The top-left panel shows the training and validation loss as a function of epoch. Both curves decrease rapidly and then flatten, and the validation loss closely follows the training loss, which indicates that the network generalizes well and does not overfit. The remaining panels compare the abundances predicted by the network with those computed by UCLCHEM for the test set. For every species the predictions lie close to the one-to-one relation across the full range of abundances, with only a small number of outliers near the edges of the parameter space. This confirms that the emulator is accurate and reliable.

Appendix B: Corner plots for the CND and SSCs in NGC 1068

Fig. B.1-Fig. B.3 presents the posterior distributions of the four physical parameters (gas density, kinetic temperature, column density, and cosmic ray ionization rate) for representative regions in the CND and the starburst ring. The diagonal panels show the marginalized distribution of each parameter, while the off-diagonal panels show the pairwise correlations.

Appendix C: CS abundance as a function of ζ

Figure C.1 shows the predicted CS fractional abundance as a function of the cosmic ray ionization rate for the heating and quiescent models. The relation between X_{CS} and ζ becomes linear only at $\zeta/\zeta_0 \gtrsim 100$. Since the regions in NGC 1068 lie below this value, CS falls in the nonlinear regime and on its own does not provide a reliable constraint on ζ .

Appendix D: Posterior predictive check

To assess the goodness of fit of the Bayesian inference, we perform posterior predictive checks (PPCs) for all the subregions. A PPC generates synthetic data from the posterior distributions of the inferred parameters and compares them with the observations. If the model could capture the data, the observed values should fall within the range spanned by the predicted distributions.

For each region, we compute the predicted line ratios from the posterior distribution between the 16th and 84th percentiles. Figure D.1 presents the PPCs for the subregions of the CND, the SSCs, and the SHC on the starburst ring. In each panel, the points indicate the observed line ratios, the shaded bars show the 68% credible intervals of the posterior predictive distribution.

For most line ratios, the observed values fall within the predicted credible intervals, confirming that the model adequately reproduces the observed emission across the different environments in NGC 1068. The C_2H related ratio is noticeably less well reproduced compared to the other ratios. The posterior predictive distributions for this ratio show larger scatter and, in several regions, the observed values lie near the boundary of the error bars. This is mainly because the $\text{C}_2\text{H}(N = 1-0)$ transition consists of six hyperfine components grouped into two fine structure groups that are blended at our velocity resolution (Sect. 2.2; García-Burillo et al. 2017). The integrated intensity therefore encompasses the full $N = 1-0$ multiplet. In the radiative transfer calculation, we model C_2H using the $N = 1-0$ transition as a whole, which does not fully account for the relative

excitation of individual hyperfine components. This simplified treatment introduces additional uncertainty in the predicted C_2H intensity that propagates into the line ratio. Despite this limitation, the C_2H related ratio does not drive the inference toward systematically biased physical parameters, as demonstrated by the consistency of our results across regions where C_2H is and is not detected.

While the posterior predictive checks confirm that the model reproduces the observed line ratios within the measurement uncertainties, this does not guarantee that all physical parameters are tightly constrained by the available data, since some ratios stay nearly constant over a wide range of conditions and can be matched by many parameter combinations (Viti et al. 2014). We also use fewer species than Holdship & Viti (2022), which limits the constraining power and leaves some degeneracy between density, temperature, and column density. The hierarchical Bayesian framework can compensate for this limitation, but compared to the rich ALCHEMI dataset (Tanaka et al. 2024), the dataset used in this work is less adequate to fully overcome the potential degeneracy. Nevertheless, the derived parameter distributions should be interpreted as the best constraints obtainable with the current molecular species set rather than as uniquely determined values. Future observations that cover the starburst ring and include additional transitions of the same species, which would provide excitation constraints, are essential to better constrain the parameters.

Appendix E: Comparison with previous work

Table E.1 summarizes the molecular transitions, spatial resolutions, and methods used in previous multi-molecular studies of NGC 1068 that we compare with in Sect. 5.1. The studies differ in the set of transitions analyzed and in whether chemical modeling was included, which helps to interpret the differences in the derived physical parameters shown in Fig. 6. Viti et al. (2014) and Scourfield et al. (2020) coupled radiative transfer with UCLCHEM, whereas Butterworth et al. (2022) used radiative transfer alone. These differences in tracers and methods, together with the range of spatial resolutions, account for much of the scatter seen when comparing the inferred densities, temperatures, and ionization rates.

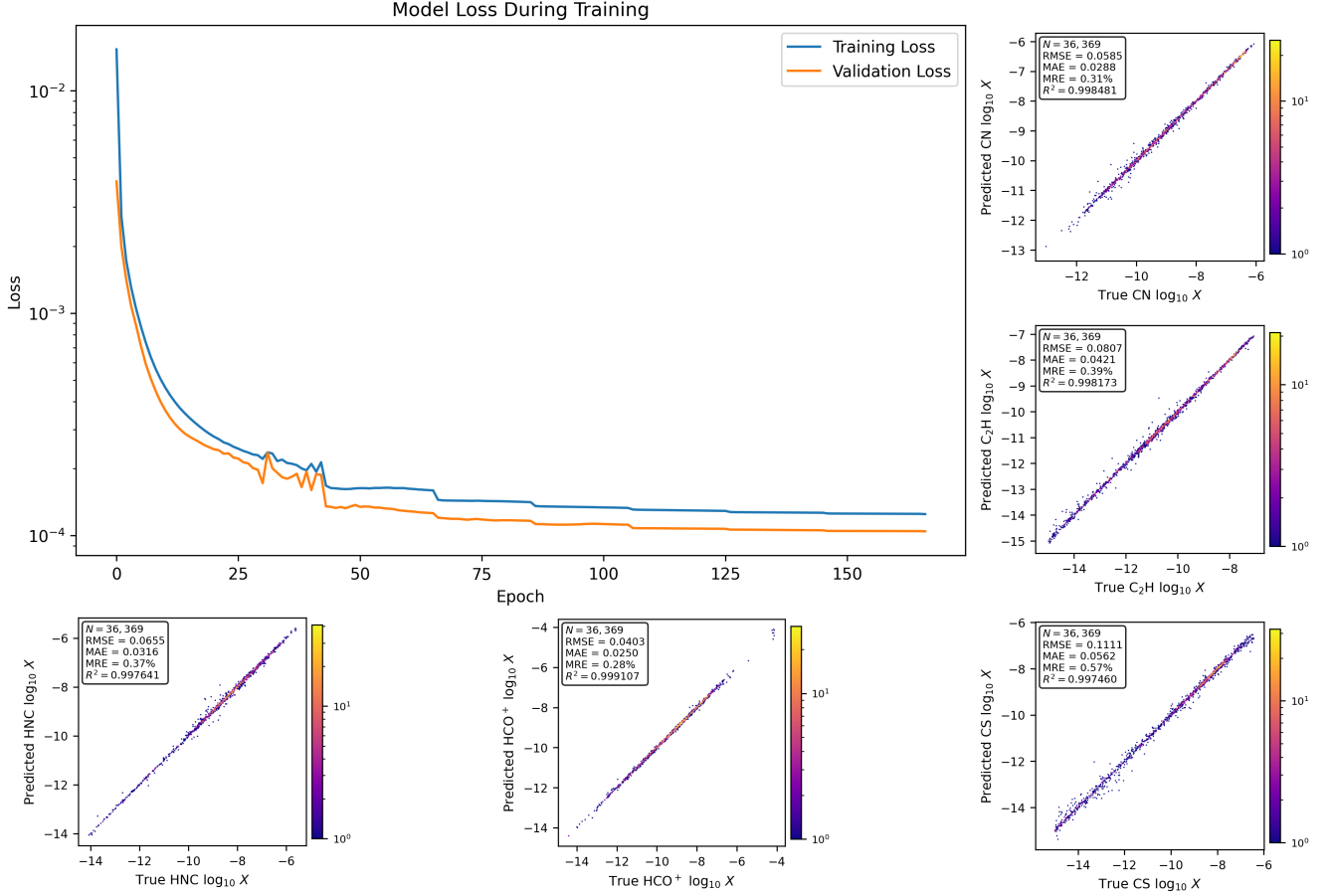


Fig. A.1: Performance of the neural network during training and testing. The top left panel shows the evolution of the training and validation loss as a function of epoch. The remaining panels compare the predicted and UCLCHEM-derived abundances for the molecules used in this work, illustrating the accuracy of the trained model across the full dynamic range of abundances.

Table E.1: Summary of molecular transitions and methods used in previous multi-molecular studies of NGC 1068.

Study	Transitions used	Resolution	Methods
Viti et al. (2014)	CO(1–0), CO(2–1), CO(3–2), CO(6–5) HCN(1–0), HCN(4–3) HCO ⁺ (1–0), HCO ⁺ (4–3) CS(2–1), CS(7–6)	~100 pc	Non-LTE RADEX grids + UCLCHEM
Scourfield et al. (2020)	CS(2–1), CS(3–2), CS(6–5), CS(7–6)	~35 pc	RADEX χ^2 fitting coupled with UCLCHEM
Butterworth et al. (2022)	HCN(1–0), HCN(4–3) HCO ⁺ (1–0), HCO ⁺ (4–3) CS(2–1), CS(7–6)	~40 pc	Non-LTE RADEX with MCMC sampling. No chemical modeling.

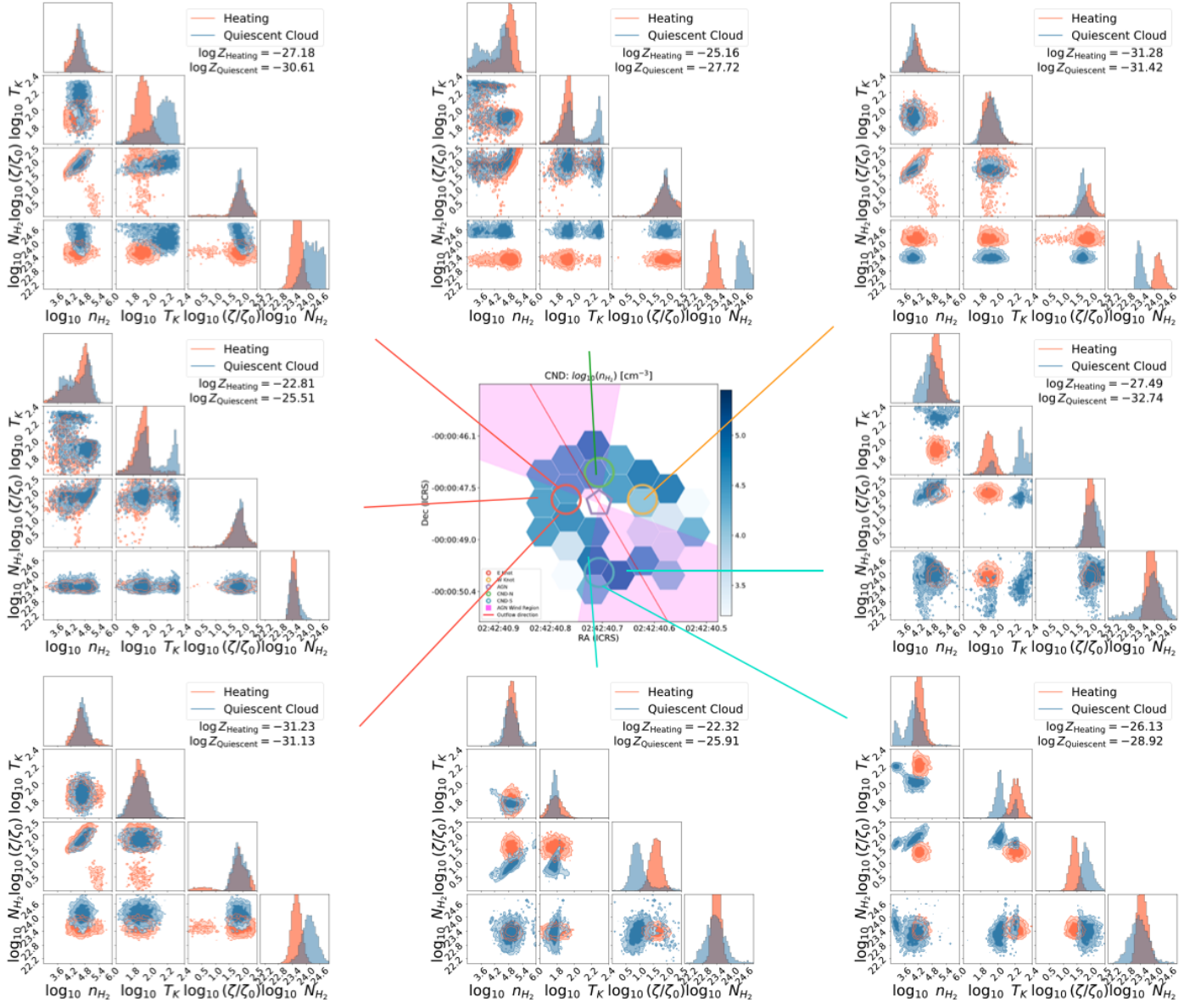


Fig. B.1: Corner plots of the posterior distributions of the physical parameters in each hexagonal region of the CND. The central panel shows the hexagonal sampling grid, with the colored circles marking the regions for which the corner plots are displayed. Orange points and histograms correspond to the heating model and blue ones to the quiescent cloud model.

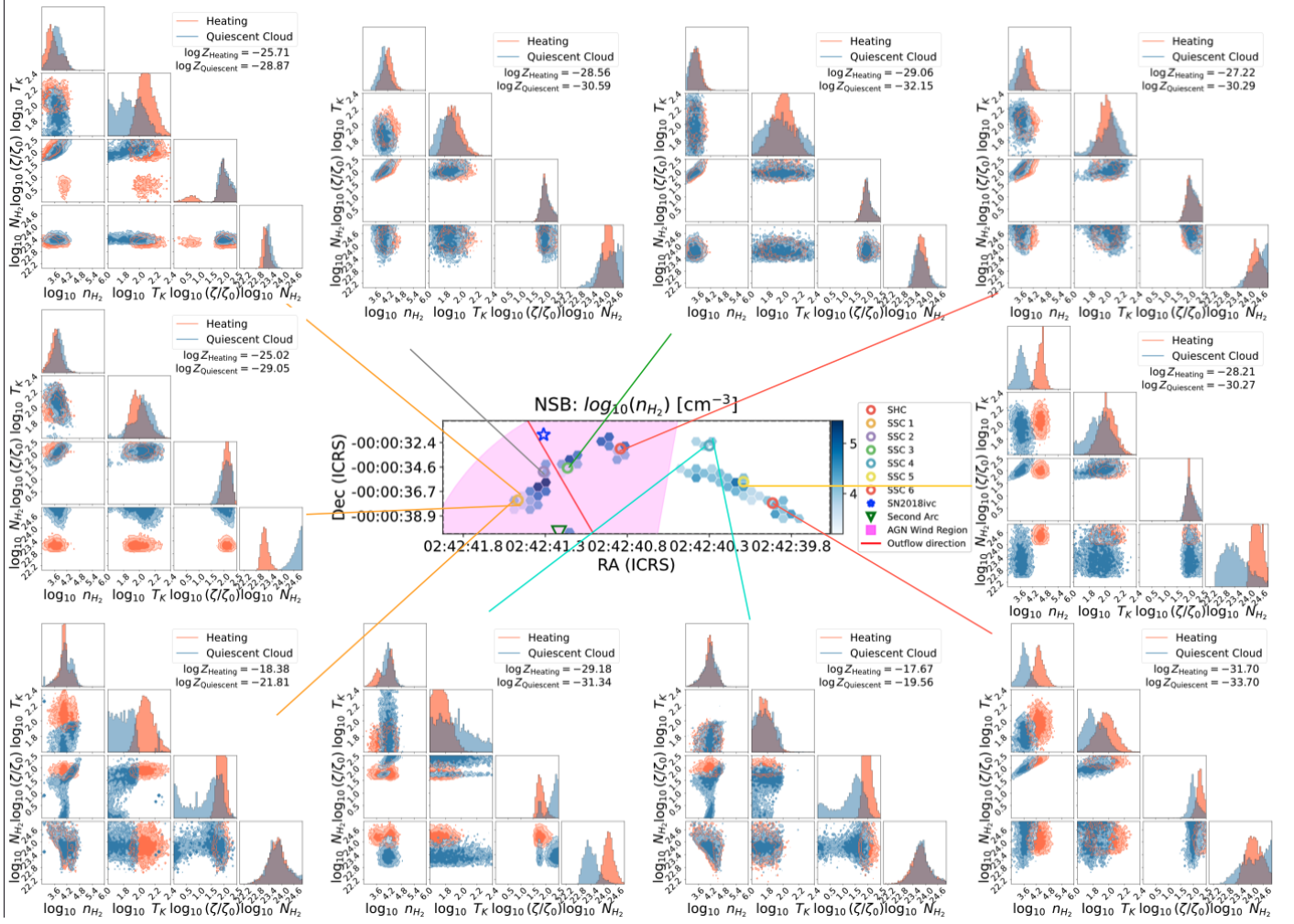


Fig. B.2: Same as Fig. B.1, but for the northern starburst ring.

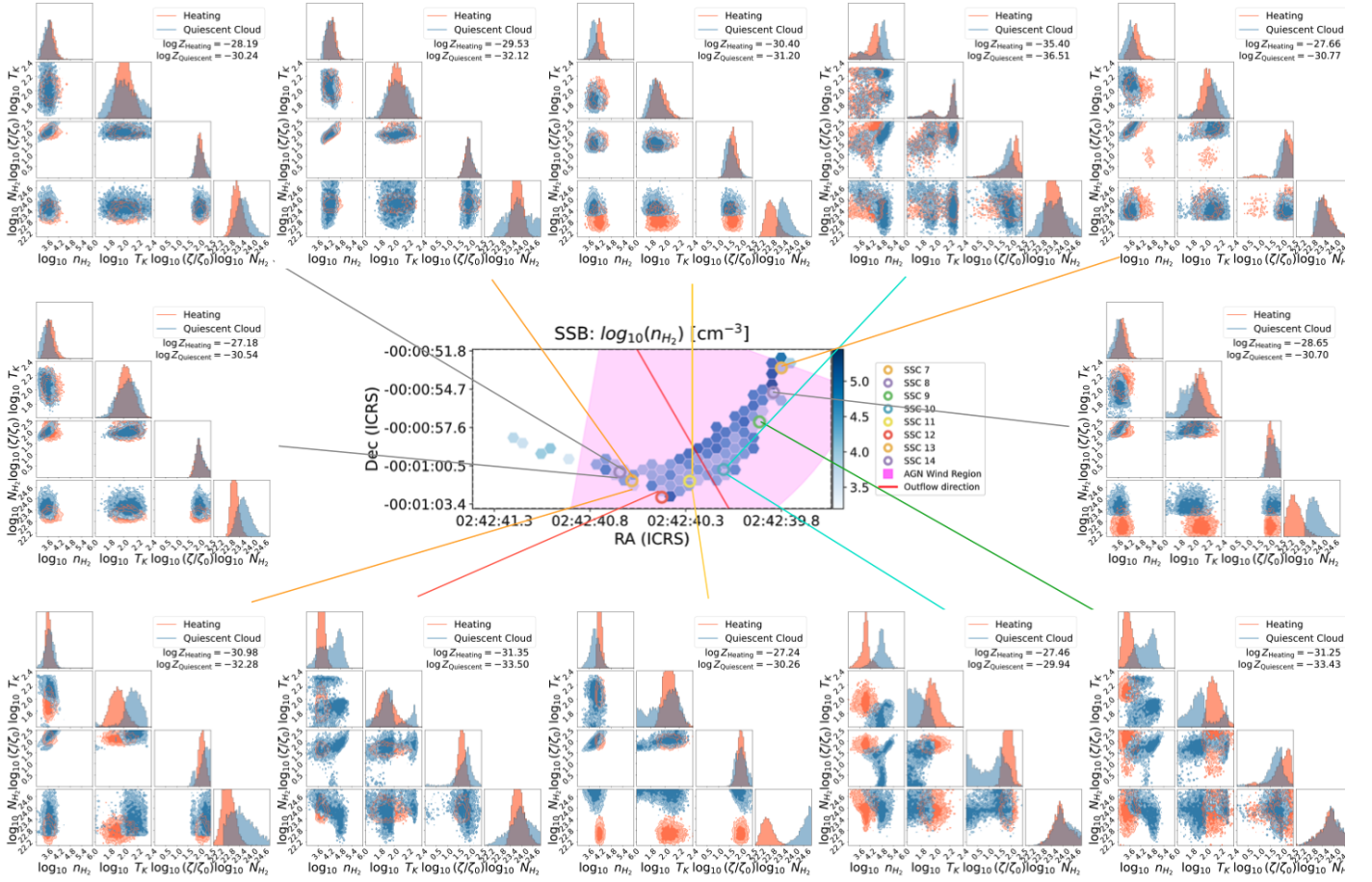


Fig. B.3: Same as Fig. B.1, but for the southern starburst ring.

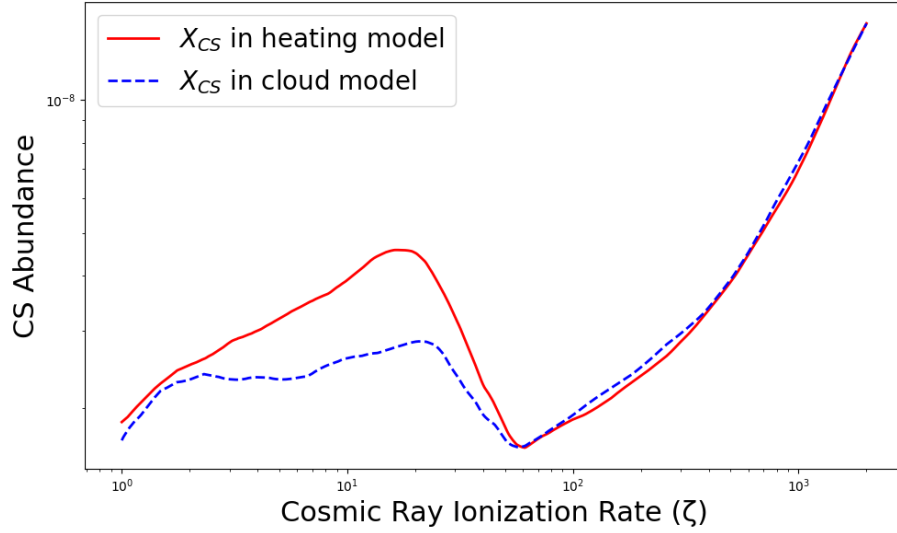


Fig. C.1. CS abundance as a function of cosmic ray ionization rate, using $n_{H_2}=10^4 \text{ cm}^{-3}$ and a temperature of 70 K, which represents an average physical condition in NGC 1068. The solid red line represents the CS fractional abundance (X_{CS}) in the heating model, while the dashed blue line shows X_{CS} in the quiescent cloud model. Both models show a linear relation at high cosmic ray ionization rates ($\zeta > 100\zeta_0$), but for lower CRIR regime, X_{CS} variation suggests that it is not a good tracer alone.

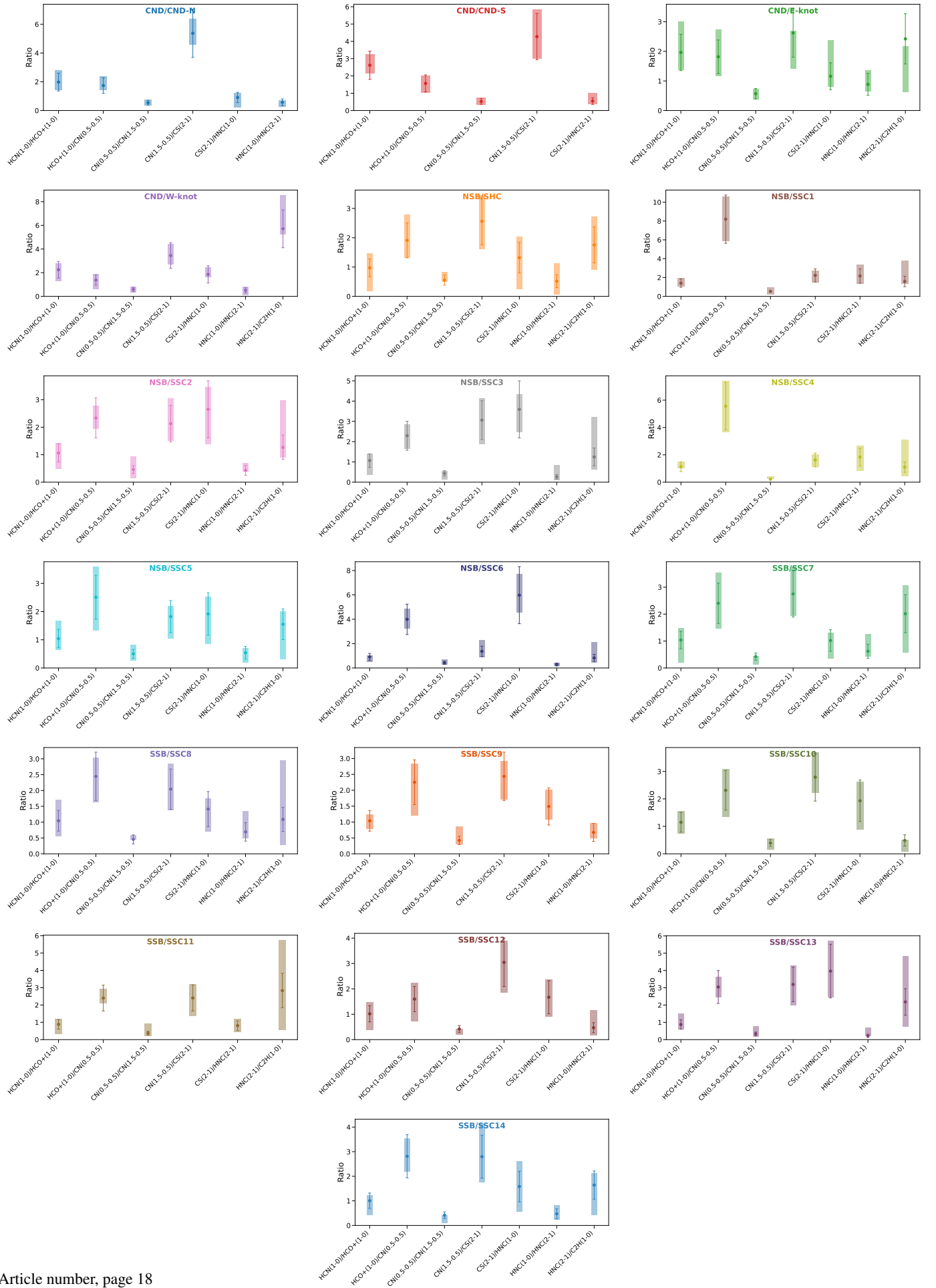


Fig. D.1: Posterior predictive checks for the subregions of the CND, the SSCs and the SHC on the starburst ring.