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# ESTIMATION OF THE PHYSICAL CONDITIONS IN PDRS FROM IGRINS RO-VIBRATIONAL $H_2$ OBSERVATIONS

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**Abstract.** $H_2$ ro-vibrational lines emitted from photon dominated regions (PDRs) serve as a powerful tool to probe the physical and microphysical processes in this interface between HII regions and molecular clouds. Thanks to the unprecedented observations from IGRINS in 2021, more than 100 emission lines have been detected in 5 different PDRs, going up to v=13 and J=10. We compare the observations to grids of Meudon PDR models to assess the ability of PDR models to explain these newly observed constraints, and to estimate the physical conditions in these 5 PDRs. By leveraging a detailed consideration of processes impacting $H_2$-such as collisions or chemical reactions-the models are able to reproduce over 85% of the detected lines within a factor of two. The $H_2$ ro-vibrational lines are found to be able to constrain the physical parameters (thermal pressure $P_{th}$ and $G_0$) as well as on microphysical parameters such as the distribution in quantum levels at formation. By adding additional constraints, we were able to fully constrain the parameters and derive uncertainties. Ultimately, the ro-vibrational lines of $H_2$, now widely observed with JWST, are well-reproduced by current state-of-the-art PDR models. These highly excited lines, emitted in the warmer regions close to the $H/H_2$ transition, yield a physical picture of PDRs that remains consistent with findings from other warm molecular tracers.

Keywords: Infrared – ISM – lines and bands – photon-dominated regions (PDR) – Orion Bar – Horsehead nebula – S140 – IC63 – NGC2023 Techniques: spectroscopy, Methods: models, data analysis, Bayesian method, neural networks

## 1 Introduction

The impact of the radiative feedback from young massive stars on their parent molecular cloud and on stellar formation remains poorly constrained. Intense stellar illumination of molecular clouds generates photodissociation regions (PDRs), which host a wide range of complex physical, chemical, and microphysical processes. The UV flux from these stars dissociates molecules and heats the gas, thereby reducing the cloud's molecular reservoir. Simultaneously, it can compress the clouds due to the evaporation dynamics of the ionization front.

Therefore, studying PDRs and constraining their key parameters is a crucial step toward understanding the impact of stellar radiative feedback on star formation. Recent instruments like NIRSpec (Peeters et al. 2024; Van De Putte et al. 2024), ALMA (Goicoechea et al. 2019) or IGRINS (Kaplan et al. 2021) allow unprecedented detections of new tracers (high ro-vibrational $H_2$, vibrationally excited CO, $CH_3^+$,...) originating from PDRs, allowing us to probe different depths and unveil the processes occurring at the interface.

This paper uses unprecedented observations of numerous ro-vibrational $H_2$ emission lines (up to v=13, J=10) detected by the IGRINS ground-based spectrometer (Kaplan et al. 2021) in 5 different PDRs: the Orion Bar, the Horsehead Nebula, NGC2023, S140 and IC63 and compares them with models from the Meudon PDR code (Le Petit et al. 2006) to derive the main physical parameters (UV field intensity: $G_0$ and thermal pressure of the gas: $P_{th}$) and microphysical processes of PDRs.

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## 2 Data & Methods

We utilize observations from Kaplan et al. (2021), incorporating two notable updates: the data have been calibrated in flux and the correction of the extinction has been updated. On the basis of their incident UV field, the five observed PDRs can be divided into two categories: three are moderately illuminated (S140, IC63, Horsehead), with an expected $G_0$ on the order of a few hundred, one is intermediate (NGC2023 with an expected $G_0$ of a fe thousands while the fifth is the Orion Bar, an intense PDR with a high star formation rate and an expected $G_0$ of at least 10,000.
We compare these data to models from the Meudon PDR code, following the prescriptions outlined in Joblin et al. (2018) for the dust distribution, $R_V$, or elementary abundances varying only the UV field intensity and thermal pressure. We create a grid of models with $G_0$ ranging from 10 to $10^5$ and $P_{th}$ from $5 \times 10^5$ to $5 \times 10^9$ K$\times cm^{-3}$. A third parameter is added : $\Omega$ the scaling factor, to take into account different geometrical aspects as detailed in Sheffer et al. (2011). Each PDR was modeled with a specific incident radiative field, which used a stellar spectrum from the Pollux database (Palacios et al. 2010a) of theoretical spectra that matched the primary illuminating star of the PDR.
Using two complementary approaches, a $\chi^2$ minimization and a Bayesian inversion (Palud et al. 2025), we explored the parameter space to deduce which model best represents the observations, and therefore, to constrain the parameters. The advanced Bayesian inversion method allows to explore the posterior in order to quantify the uncertainties of the best fitting model derived.

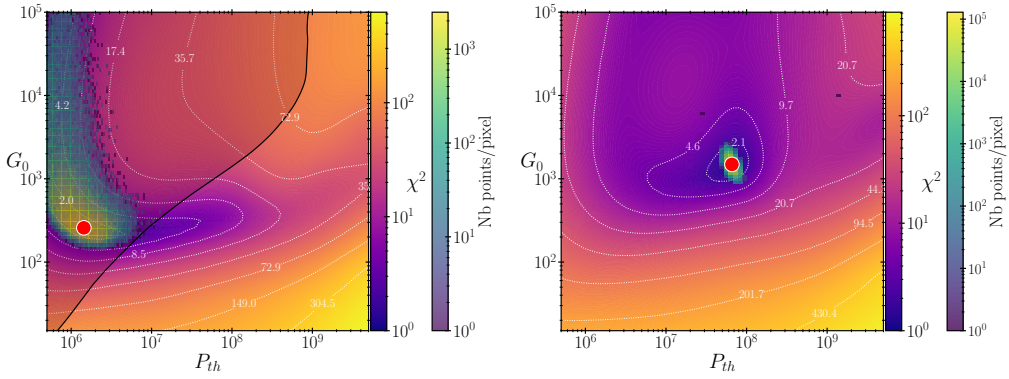
## 3 Results

The exploration of the parameter space successfully constrained the PDRs, revealing a behavioral difference between moderate and intense PDRs.
For the moderate PDRs, the observed lines are sensitive to variations in thermal pressure and the incident UV field strength as few models correctly reproduce the observations. However, we consistently find an L-shaped minimum in the $\chi^2$ map (as shown in Fig. 1), which indicates a slight degeneracy between the parameters. To reduce these uncertainties and select the most relevant model, additional constraints were applied, such as incorporating pure rotational lines for NGC2023 (Sheffer et al. 2011) and a maximum distance limit for the H/$H_2$ transition in the case of the Horsehead nebula (Hernández-Vera et al. 2023). These constraints systematically guide the selection toward the best model within the high-pressure branch of the degeneracy. Figure 2 presents an excitation diagram for the Horsehead Nebula, showing the observations with error bars and the best-fit models both with and without additional constraints. Ultimately, the best models for each moderate PDR reproduce over 85% of the detected lines within a factor of two, with a reduced $\chi^2$ of less than 2. This demonstrates the Meudon PDR code's ability to capture the essential processes and accurately reproduce the physics of these complex regions.
On the other hand, for the intense PDRs in this dataset, represented by the Orion Bar, we observe a lower sensitivity of the lines to the two parameters, as shown in Fig. 1. The addition of a minimal $G_0$ constraint (Van De Putte et al. 2024)allows for a proper estimation and constraint of both the thermal pressure and the UV field intensity.

Thanks to this study of $H_2$ ro-vibrational lines and the inclusion of supplementary constraints, we can effectively constrain both $P_{\rm th}$ and $G_0$ in moderately illuminated PDRs.
The large number of detected ro-vibrational lines also enables us to study the various microphysical processes at work within the PDR. For the first time, we observed a sensitivity to the initial quantum level distribution at formation of $H_2$ on dust surfaces by comparing two identical models that differed only in their formation distribution prescription. When comparing a Boltzmann distribution at the gas temperature to an advanced prescription proposed in Sizun et al. (2010), we observed a notable difference for the moderate PDRs, primarily at v=1 and high J levels, as seen in Fig. 3. This improved modeling of moderate PDRs using the Sizun prescription confirms that $H_2$ molecules, when desorbing from grain surfaces, preferentially form with high vibrational rather than rotational energy.

## 4 Conclusion

We have compared $H_2$ ro-vibrational emission lines coming from five different PDRs with grids of models generated by the Meudon PDR code to estimate the main physical parameters $G_0$ and $P_{th}$ and micro physical




(a) Horsehead Nebula (b) Orion Bar

Fig. 1: $\chi^2_R$ contour map (blue-green color bar) in the $P_{\rm th} - G_0$ plane at best $\Omega$ for each PDR with superimposed a 2D histogram of the posterior samples, generated with the MCMC algorithm implemented in BEETROOTS (purple-yellow color bar). The red point represents the best-fit model found with the $\chi^2_R$ minimisation and BEETROOTS. For the Horsehead nebula, the constraint on the maximum distance of the H/$H_2$ transition to the ionization front, at 650 AU is highlighted in black. For the Orion Bar, an addition constrain, $G_0 \geq 10^4$, is represented by the black line. All modeled distances beyond this threshold are shaded. For the PDRs for which additional constraints are considered, the best proposed model is represented with a green cross.

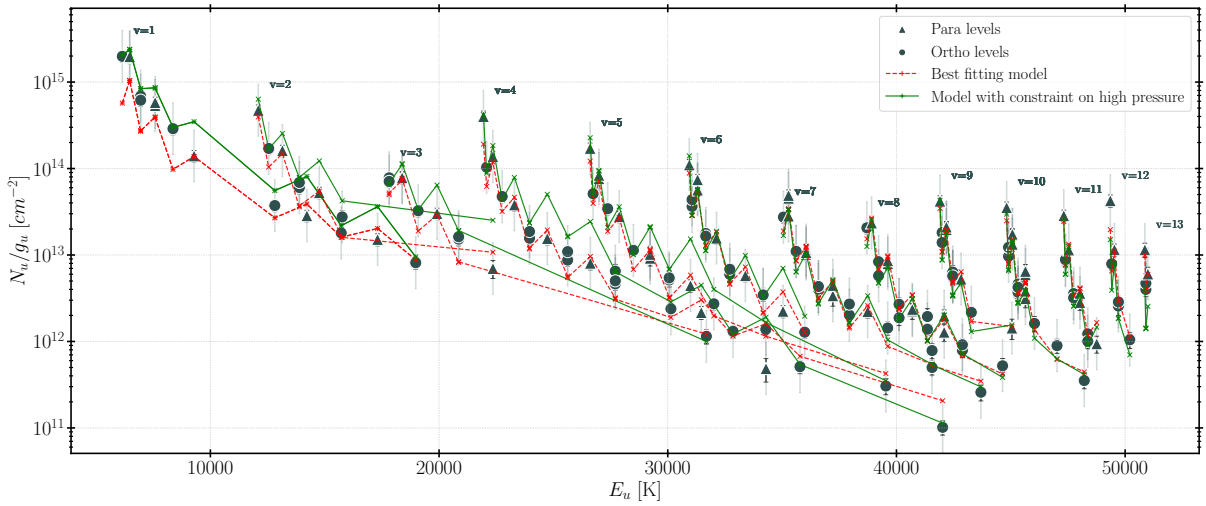



Fig. 2: NGC2023 Excitation diagram with IGRINS observations in dot (ortho levels) and triangles (para levels) with observational uncertainties from modeling uncertainties and in semi-transparent the error bars within a factor of 2. In red plain line is the best fitting model (red dot in Fig. 1). In green the most relevant model taking into account the constraints favoring the high-pressure branch to the high UV illumination branch.

processes impacting $H_2$ level distribution.

The PDR Meudon code effectively constrains the physical parameters of PDRs, thanks to the extensive number of $H_2$ emission lines, resulting in only small regions of acceptable parameter space. These regions can be further refined by incorporating additional constraints through stronger priors on the parameters and by selectively sampling the posterior based on other observables such as the H/$H_2$ transition distance. Using this approach, we propose pertinent models for each PDR, fitting over 90% of the $H_2$ lines observed by IGRINS within a factor of 2, and achieving overall agreement with values reported in the literature.

Thanks to a detailed modeling of multiple mechanisms in the PDR, the PDR Meudon code can reproduce most of the $H_2$ line intensities observed by IGRINS. Key improvements include: detailed modeling of $H_2$ through its excitation processes and its variations according to the intensity of the UV field, and detailed modeling of

Table 1: Best fitting models for each PDR issued from Bayesian inversion. The uncertainties are detailed in the article. Each PDR is modeled with a specific illuminating stellar spectrum.

| **PDR** | S140 | IC63 | Horsehead | NGC2023 | Orion Bar |
|---|---|---|---|---|---|
| $G_0$ | 504 | 542 | 258 | 1,018 | 10,280 |
| $P_{\rm th}[K\,cm^{-3}]$ | $9.5 \times 10^5$ | $2.5 \times 10^6$ | $6.3 \times 10^6$ | $5 \times 10^7$ | $5.2 \times 10^7$ |
| $\Omega$ | 9.8 | 3.5 | 8.1 | 9.9 | 4.2 |
| $\chi^2_R$ | 1.7 | 1.7 | 3.8 | 4.4 | 5 |
| Lines within a factor of 2 | 95% | 95% | 92% | 85% | 86% |

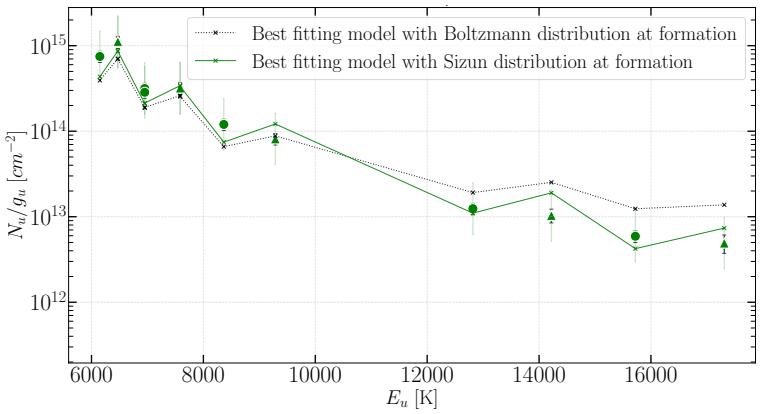



Fig. 3: $H_2$ excitation diagram for v = 1 for S140. The dots represent IGRINS observations. Comparison between the "Boltzmann distribution" and the distribution suggested in Sizun et al. (2010)

spectral shape and orientation of stellar illumination of the PDR.
This unique dataset allows, for the first time, the observation of the impact of the initial $H_2$ ro-vibrational distribution upon formation on $H_2$ emission lines: the prescription from Sizun et al. (2010) leads to a decrease in modeled intensities at high J for v=1, enabling improved modeling of moderate PDRs.

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## References

Goicoechea, J. R. et al. 2019, A&A, 622, A91
Van De Putte, D. et al. 2024, A&A, 687, A86
Peeters, E. et al. 2024, A&A, 685, A74
Joblin, C. et al. 2018, A&A, 615, A129
Le Petit, F. et al. 2006, ApJS, 164, 506
Kaplan, K. F. et al. 2021, ApJ, 919, 27
Sizun, M. et al. 2010, Chemical Physics Letters, 498, 32
Palud, P. et al. 2025, arXiv e-prints, arXiv:2504.08387
Sheffer, Y. et al. 2011, ApJ, 741, 45
Hernández-Vera, C. et al. 2023, A&A, 677, A152
Palacios, A. et al. 2010a, A&A, 516, A13
Palacios, A. & Gebran, J. 2010b, The Pollux data base (http://pollux.oreme.org/)