

Multi-line Observations, Models, and Data Needed to Understand the Nature of UV-irradiated Interstellar Matter

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Abstract. Far-ultraviolet photons from OB-type massive stars regulate the heating, ionization, and chemistry of much of the neutral interstellar gas in star-forming galaxies. The interaction of FUV radiation and interstellar matter takes place in environments broadly known as *photodissociation regions* (PDRs). PDR line diagnostics are the smoking gun of the radiative feedback from massive stars. Improving our understanding of stellar feedback in the ISM requires quantifying the energy budget, gas dynamics, and chemical composition of PDR environments. This goal demands astronomical instrumentation able to deliver multi-line spectroscopic images of the ISM (of the Milky Way and nearby galaxies). It also requires interdisciplinary collaborations to obtain the rate coefficients and cross sections of the many microphysical processes that occur in the ISM and that are included in models such as the *Meudon* PDR code.

1 Introduction

Far-UV (FUV: $E < 13.6$ eV) photons emitted by massive O- and B-stars govern, or at least greatly influence, the heating, ionization, and chemistry of the neutral interstellar gas: everywhere hydrogen atoms are in predominantly neutral form. The interaction of stellar FUV radiation and interstellar baryonic matter (atoms, molecules, and dust grains) takes place in so-called *photodissociation regions* (PDRs; [1]). This interaction occurs for different doses of FUV radiation (G_0) and at very different spatial scales: from the illuminated rims of star-forming clouds to kpc scales in starburst galaxies. The emission from PDRs reflects the radiative feedback from massive stars, a collection of processes that establish the phases and pressures of the ISM, and also regulate star formation and molecular cloud destruction [2].

The physical state of the interstellar gas depends on a plethora of detailed microphysical processes that determine its chemical composition and how the gas is heated and cooled. Therefore, in addition to understanding the (macro) astrophysical processes driving the dynamics and evolution of the ISM, it is also mandatory to understand the subtle microprocesses that form, destroy, and excite its basic constituents. Accompanied by new developments in astronomical instrumentation, last years on PDR research have reinforced closer collaborations with molecular physicists and laboratory experimentalists able to determine the rate coefficients and cross sections of the relevant microprocesses.

Bright molecular cloud rims, such as the iconic Orion Bar or the Horsehead, have always been excellent laboratories to study the molecular content of FUV-irradiated interstellar gas

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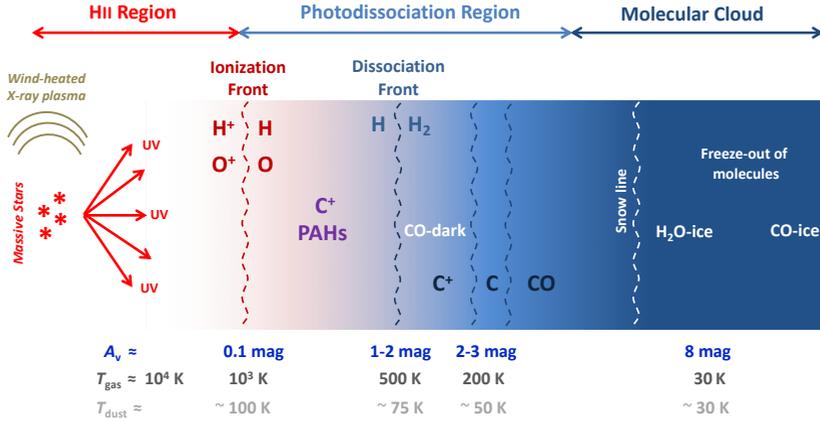


Figure 1. Structure of a strongly irradiated molecular cloud near massive stars (e.g., the Orion Bar).

and the wealth of physical and chemical processes that occur at microscopic (molecular) level. The number of molecules, atoms, and ions observed in these dense PDRs are not so easily detected toward fainter environments also influenced by stellar FUV radiation (e.g, the surface layers of protoplanetary disks and distant star-forming galaxies).

In this invited paper we summarize some of the latest developments in observations and modeling of PDRs. Due to the lack of space, we mostly limit to our own recent work. Readers are referred to Wolfire *et al.* [3] for a modern review on PDRs. Here we strengthen the interdisciplinary aspects of PDR research, and we emphasize the need of precise atomic and molecular data to correctly interpret future observations of the ISM in galaxies.

2 PDRs everywhere

PDRs host the critical conversion from atomic to molecular gas (the H/H₂ and C⁺/C/CO transition zones, Fig. 1). This stratification occurs as the column density of gas and dust increases deeper inside molecular clouds, and as the flux of FUV photons is attenuated by dust (for high G_0/n_H ratios) and by H₂ absorption lines (for low G_0/n_H ratios) [4]. The penetration of FUV radiation depends on metallicity and grain properties. FUV photons reach larger depths in lower metallicity environments (lower dust-to-mass ratios) and in regions affected by grain growth (flatter extinction curves). Both effects shift the C⁺/C/CO transition to higher A_V and leave a larger mass fraction of H₂ gas that is “CO-dark” (or too faint).

PDRs emit most of the IR radiation arising from the ISM of star-forming galaxies: FUV-pumped IR bands from polycyclic aromatic hydrocarbons (PAHs), H₂ ro-vibrational, [C II]158 μm and [O I]63, 145 μm fine-structure, and mid- J CO lines, as well as warm dust continuum – grains are heated by FUV photons and reemit FIR continuum. Photoelectrons ejected from small grains and PAHs heat the gas. In dense PDRs, collisional de-excitation of FUV-pumped H₂ is an important gas heating mechanism too. The presence of vibrationally excited H₂($v \geq 1$) overcomes the endoergicity of the initiating reactions H₂ + (C⁺, S⁺, O, N, ...) [5] and leads to the formation of CH⁺, SH⁺, OH, and NH [6].

In their most general definition – *neutral gas regulated by FUV radiation* –, PDRs represent the dominant fraction of the neutral atomic and molecular gas in the ISM of star-forming galaxies [1, 3]. Indeed, except for the cold and dense molecular cores associated with the first stages of star formation, most of the ISM (in volume and mass) is effectively at $A_V < 8$ mag. Hence, permeated by stellar FUV photons.

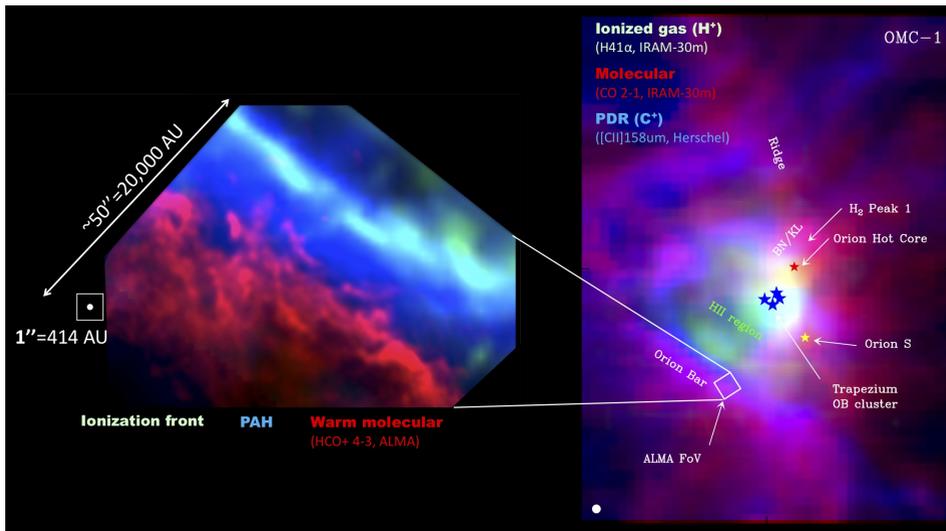


Figure 2. Central parsec ($\sim 7.5' \times 11.5'$) of the Orion molecular core OMC-1 around the Trapezium cluster (*right*, [7]) and $1''$ resolution zoom ($\sim 50'' \times 50''$) resolving a high pressure ($P_{\text{th}}/k_{\text{B}} \sim 10^8 \text{ K cm}^{-3}$) and nearly edge-on H II/PDR/molecular cloud interface in the Orion Bar PDR (*left*, [8]).

2.1 New-generation observations of the ISM and PDR environments

State-of-the-art observations allow us to access a plethora of multi-line diagnostics at increasingly higher sensitivity, angular resolution, and field-of-view. Recent observations challenge some of our previous views of PDRs, for example, their fundamental small-scale structure(s), the origin of the observed rich chemistry, and their gas dynamics: propagation of ionization/dissociation fronts, photoevaporation, gas compression, and radiation pressure on grains. Last years have seen rapid progress in heterodyne receiver technology and specific techniques involving (sub)mm spectral-imaging of the ISM:

i) Increased sensitivity and angular resolution of interferometric mosaics (with ALMA and NOEMA), providing astonishing sub-arcsecond resolution images of the fundamental structure of the ISM (e.g., see Fig. 2 for the Orion Bar PDR [8]).

ii) Broader instantaneous bandwidth, allowing us to *a)* map large portions of star-forming clouds in several molecular lines simultaneously (CO, HCN, HNC, HCO^+ , N_2H^+ , ... [9]), and *b)* to obtain deep line surveys of the molecular content (through the detection of hundreds of molecular lines [10, 11]) and physical conditions of representative environments. IRAM, its forefront instrumentation, and the variety of available observational techniques (from on-the-fly mapping to line surveys) have played a pivotal role in improving our understanding of the ISM and its underlying PDR processes.

iii) Development of airborne multi-pixel arrays up to the THz domain, able to map the main gas cooling lines (i.e., the cloud energetics) at high-spectral resolution and providing, for example, velocity-resolved square-degree maps of the $[\text{C II}]158 \mu\text{m}$ emission [2].

As a consequence of these developments, current research on PDRs and associated processes is not only about the detailed study of small fields in bright cloud rims such as the Orion Bar – from which we learn so much – but more generally about the role of stellar feedback and the evolution of the FUV-illuminated ISM at all relevant spatial scales: from cores and giant molecular clouds (GMCs) [2, 7] to distant star-forming galaxies.

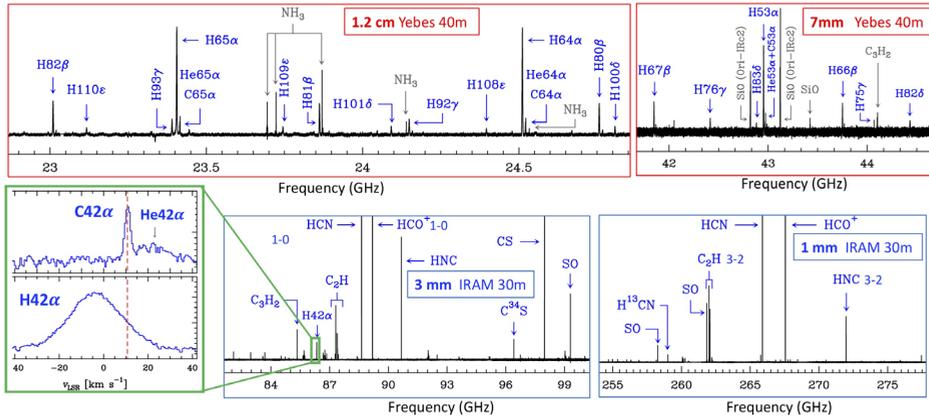


Figure 3. Multi-line diagnostics (molecular and recombination lines) observed toward the Orion Bar PDR and adjacent H II region using the IRAM 30m [10–12] and Yebes 40m [18] radiotelescopes.

2.2 Molecular content of PDRs and peculiarities

PDRs were once thought to be too harsh to develop a rich chemistry. However, our IRAM 30m and Yebes 40m line surveys of the Orion Bar, a strongly irradiated PDR ($G_0 \approx 10^4$), exemplify that PDRs do host multiple lines and unique chemical features that are not seen (or are too faint to be detected) in regions shielded from FUV radiation. These specific lines (Fig. 3) have a great diagnostic power as tracers of FUV radiation from short-lived massive stars, and thus, of star formation: narrow carbon radio recombination lines (with line intensities proportional to $n_e^2 T_e^{-1.5}$) tracing the presence of C^+ ions and of high ionization fractions ($n_e/n_H \approx C^+/H$; [12]), reactive molecular ions (CH^+ , SH^+ , HOC^+ , and CO^+ ; [13, 14]), as well as enhanced abundances of certain hydrocarbons (C_3H^+ , $l-C_3H$; [10]), radicals (NH [6], OH [11], and HCO [15]), and unstable isomers of organic molecules (*cis*-HCOOH; [16]). In addition, specific sulfur-bearing molecules such as H_2S show bright emission lines and enhanced abundances (as revealed by the detection of the rare $H_2^{33}S$ isotopologue; [17]). Indeed, the detection of sulfur radio recombination lines [18] implies a gas-phase S^+/H abundance of $(1.4 \pm 0.4) \cdot 10^{-5}$ at edge of the Orion Bar. This is the elemental gas-phase sulfur abundance before an undetermined fraction goes into S-bearing molecules and deplete as grain ice mantles in the cloud interior. The inferred sulfur abundance in the PDR edge matches the solar abundance [17]. It thus leaves little room for large depletions of sulfur onto rocky grains in molecular clouds.

Some of the above "PDR species" are readily detected in diffuse clouds [19] as well as in starburst galaxies [20]. These detections prove the interaction of stellar radiation with interstellar matter in different regimes of FUV flux, gas density, and spatial scale.

3 Models, need of precise atomic and molecular data, and outlook

The theoretical study and first thermo-chemical models of dense PDRs started to develop more than 50 years ago. PDR models solve the penetration of FUV radiation into molecular clouds. This includes treating the absorption of FUV photons to electronically excited levels of H, H_2 , and CO, as well as the absorption and anisotropic scattering by dust grains [21]. Among other things, the wavelength-dependent FUV ($\lambda > 911\text{\AA}$) radiation field at different cloud depths determines the rate at which low-ionization-potential atoms are ionized

Table 1. Microphysical processes relevant to the study of interstellar PDRs.

Process	Relevance	Required parameter	Methodology
Inelastic collisions with o -H ₂ , p -H ₂ , H, and e^-	Non-LTE excitation. Precise comparison with observed line intensities	Inelastic collisional rate coefficient $\gamma_{ij}(T) \sim \sigma_{ij} \cdot v$ (cm ³ s ⁻¹)	Scattering calculations. Laboratory.
Chemical reactions	Formation and destruction of molecules and PAHs	Reaction rate coefficient $k(T)$ (cm ³ s ⁻¹)	Reaction dynamics calculations. Laboratory.
Reactions with vibrationally excited H ₂ ($v \geq 1, J$)	Reactions of FUV-pumped H ₂ with atoms and molecules overcomes reaction endoergicities	State specific rate coefficient $k_{v,J}(T)$ (cm ³ s ⁻¹)	Reaction dynamics calculations. Laboratory.
Photo-ionization and dissociation of atoms, molecules, and PAHs	Photochemistry induced by stellar FUV photons	Photo cross sections $\sigma_{\text{ion}}(\lambda), \sigma_{\text{diss}}(\lambda)$ (cm ⁻²)	Experiments (e.g., synchrotron). Calculations.
Low- T_e radiative and dielectronic recombination of S ⁺ (Si ⁺ , Fe ⁺ , ...)	Defines S ⁺ /S transition. Determines recombination line spectrum	Recombination rate coefficients $k_{\text{RR,DR}}(T_e)$ (cm ³ s ⁻¹)	Calculations.
Adsorption/desorption of atoms and molecules onto/from dust grains	Freeze-out, grain surface chemistry and sublimation of atoms/molecules from dust grains	Binding energies E_b/k_B (K)	Temperature-programmed desorption experiments. Calculations.
Non-thermal desorption from grains	Photodesorption and cosmic-ray induced desorption of ice mantles	Desorption yields Y (molecule photon ⁻¹) k_{CR} (s ⁻¹)	FUV, X-ray, and particle irradiation experiments.
FUV extinction Photoelectric effect	FUV penetration. Gas heating	Grain/PAH optical props. $Q_{\text{abs}}(\lambda), Q_{\text{sca}}(\lambda), g(\lambda)$	Laboratory.

(C, S, Si, Fe, ...) and at which molecules are ionized and dissociated. The FUV field, gas density, and dust/PAH properties set the main heating mechanisms, whereas cooling from [C II], [O I], H₂, and mid- J CO emission lines [22] determines the cloud-depth variation of the gas temperature. This temperature sets the rates of a large network of gas-phase ion-neutral and neutral-neutral chemical reactions forming and destroying molecules. At deeper depths into the molecular cloud, typically $A_V > 8$ mag, the flux of stellar FUV photons is almost completely attenuated and gas-phase molecules and atoms freeze-out on dust grains as temperatures drop. Cosmic-rays drive the ionization of atoms and molecules, but at much lower rates than in gas directly exposed to stellar FUV radiation. This leads to low ionization fractions and a slower chemistry. The catalytic formation of molecules on grain surfaces and subsequent thermal (sublimation) and nonthermal (photodesorption, cosmic-ray induced, or chemical) desorption adds a new layer of chemical complexity to model.

In order to correctly interpret the amount of information and the many details provided by state-of-the-art multi-line observations, astrochemical models need to accurately calculate the rates of the above microphysical processes (interstellar gas is rarely in thermal or chemical equilibrium). This is the main goal of the *Meudon* PDR code [23], a publicly available and open source model (<https://ism.obspm.fr/>) that is continuously upgraded toward more realistic descriptions of these processes [24] and as new rate coefficients and cross sections are published in the literature. Hence, it is mandatory to strengthen and foster interdisciplinary collaborations aimed to better characterize these processes, and to determine the precise atomic and molecular data needed in astrochemical models. These data can be obtained in sophisticated laboratory experiments or through high-level *ab initio* calculations. Table 1 summarizes some of the most relevant microphysical processes taking place in the ISM (with emphasis on PDRs) together with the physical parameters and rate coefficients typically needed in accurate thermo-chemical and non-LTE excitation models.

PDR models play a central role to correctly interpret spectroscopic observations of a very significant fraction of the ISM in star-forming galaxies (all neutral gas at $A_V < 8$ mag). New instrumentation will allow mapping several square-degree areas of GMCs (reaching the scales that dominate the extragalactic emission) in multiple rotational lines, critical to derive accurate physical conditions and precise chemical abundances. More automatic statistical data analysis tools – designed to link large grids of astrochemical models and hydrodynamic PDR simulations with observations – will be used to extract all the information contained in the million spectra these velocity-resolved cubes will generate [9]. These cubes provide access to the gas kinematics, thus to the driving forces in the ISM, and reveal the dynamical and non-stationary aspects of stellar feedback in the ISM (e.g., [25]). In parallel, interferometric mosaics will allow us to locally zoom into particular fields/templates at very high angular resolution. These images reveal the spatial scales at which chemical abundances and physical conditions abruptly change in clouds (Fig. 2). Interferometric observations also spatially resolve GMCs in nearby galaxies, with emission features often dominated by gas at low A_V . JWST will soon reveal the evolution of PAHs, warm dust grains, and H_2 emission (e.g., [26]) in all kind of FUV-irradiated environments. The IR to cm emission from these “PDRs” is determined by many microphysical processes that form, excite, and destroy the gas and dust in the ISM. Knowing the rates of these processes is equally important to correctly understand the many faces of stellar feedback in the ISM.

References

- [1] Hollenbach, D. J. & Tielens, A. G. G. M. 1999, *Reviews of Modern Physics*, 71, 173
- [2] Pabst, C. H. M., Goicoechea, J. R., Teyssier, D., et al. 2020, *A&A*, 639, A2
- [3] Wolfire, M. G., Vallini, L., & Chevance, M. 2022, *ARAA*, 60, arXiv:2202.05867
- [4] Sternberg, A., Le Petit, F., Roueff, E., et al. 2014, *ApJ*, 790, 10
- [5] Agúndez, M., Goicoechea, J. R., Cernicharo, J., et al. 2010, *ApJ*, 713, 662
- [6] Goicoechea, J. R. & Roncero, O. 2022, *A&A*, arXiv:2206.10441
- [7] Goicoechea, J. R., Teyssier, D., Etxaluze, M., et al. 2015, *ApJ*, 812, 75
- [8] Goicoechea, J. R., Pety, J., Cuadrado, S., et al. 2016, *Nature*, 537, 207
- [9] Pety, J., Guzmán, V. V., Orkisz, J. H., et al. 2017, *A&A*, 599, A98
- [10] Cuadrado, S., Goicoechea, J. R., Pilleri, P., et al. 2015, *A&A*, 575, A82
- [11] Cuadrado, S., Goicoechea, J. R., Cernicharo, J., et al. 2017, *A&A*, 603, A124
- [12] Cuadrado, S., Salas, P., Goicoechea, J. R., et al. 2019, *A&A*, 625, L3
- [13] Nagy, Z., Van der Tak, F. F. S., Ossenkopf, V., et al. 2013, *A&A*, 550, A96
- [14] Goicoechea, J. R., Cuadrado, S., Pety, J., et al. 2017, *A&A*, 601, L9
- [15] Goicoechea, J. R., Joblin, C., Contursi, A., et al. 2011, *A&A*, 530, L16
- [16] Cuadrado, S., Goicoechea, J. R., Roncero, O., et al. 2016, *A&A*, 596, L1
- [17] Goicoechea, J. R., Aguado, A., Cuadrado, S., et al. 2021, *A&A*, 647, A10
- [18] Goicoechea, J. R. & Cuadrado, S. 2021, *A&A*, 647, L7
- [19] Gerin, M., Liszt, H., Neufeld, D., et al. 2019, *A&A*, 622, A26
- [20] Fuente, A., García-Burillo, S., Usero, A., et al. 2008, *A&A*, 492, 675
- [21] Goicoechea, J. R. & Le Bourlot, J. 2007, *A&A*, 467, 1
- [22] Joblin, C., Bron, E., Pinto, C., et al. 2018, *A&A*, 615, A129
- [23] Le Petit, F., Nehmé, C., Le Bourlot, J., et al. 2006, *ApJS*, 164, 506
- [24] Bron, E., Le Bourlot, J., & Le Petit, F. 2014, *A&A*, 569, A100
- [25] Maillard, V., Bron, E., & Le Petit, F. 2021, *A&A*, 656, A65
- [26] Berné, O., Habart, É., Peeters, E., et al. 2022, *PASP*, 134, 054301