

Introduction to PDR's

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PDR stands for
 Photo-Dissociation Region
 Photon Dominated Region



Wolfgang Brandner (JPL/IPAC), Eva K. Grebel (University of Washington), You-Hua Chu (University of Illinois, Urbana-Champaign) and NASA

- A region where far-ultraviolett (FUV: 6-13.6 eV) photons from young, massive stars dominate the physics and the chemistry of the interstellar medium.
 - 6 eV (2066 Å) ~ionization potential of dust/PAHs 11.1 eV (1117 Å) dissociation energy of CO 11.3 eV (1097 Å) ionization potential of C
 13.6 eV (912 Å) ionization potential of H ionization potential of O 14.5 eV (855 Å ionization potential of N

 A region where far-ultraviolett (FUV: 6-13.6 eV) photons from young, massive stars dominate the physics and the chemistry of the interstellar medium.



massive stars emit a significant fraction of their energy at $\lambda < 912$ Å

 A region where far-ultraviolett (FUV: 6-13.6 eV) photons from young, massive stars dominate the physics and the chemistry of the interstellar medium.



PDRs close to an OB star experience spectrally different UV radiation compared to the standard mean FUV field (Draine '78, Habing '68)

Interstellar PDRs include:

- Diffuse WNM and CNM clouds.
- Translucent clouds: $A_V < 5$, $n_H < 1000$ cm⁻³, weak interstellar FUV fields.
- Dense molecular clouds: A_V up to ~10, n_H > 1000 cm⁻³ including intense FUV fields near OB stars

 \rightarrow

~90% of the Galactic molecular ISM may be "photon- dominated".

Ring nebula



Speck et al. 2003 PASP 115, 170

Credit: NASA, ESA, and F. Paresce and R. O'Connell



PDRs are also observed in extragalactic source

30 Doradus in the LMC

Credit: ESA/Hubble & NASA



PDRs are also observed in extragalactic source

Antennea galaxies (NGC 4038/39)

Thilker et al. 2005



PDRs are also observed in extragalactic source

M33





Motte et al. 2010

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Basic structure



Controlling parameters:

1) cloud density/pressure

2) FUV intensity

3) grain scattering properties

4) H₂ formation rate coefficient

5) geometry/clumpiness

6) gas phase abundances

7) magnetic field

8) cosmic ray ionization

9) turbulence

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Sternberg & Dalgarno 1995

FUV

6-13.6 eV

Physical structure

- Temperature
 - heating
 - cooling
- Density
- Geometry
- Dynamics





Gas heating

- 1. FUV photons
 - 1. Photoelectric heating
 - 2. vibrational deexcitation of electronically pumped H₂
 - 3. H_2 formation heating
 - 4. gas-grain collisions
 - 5. photodissociation of H_2
 - 6. ionization of atomic carbon
- 2. Cosmic rays/X-rays
- 3. Shocks (\rightarrow Talk by A. Gusdorf)
- 4. Turbulence

Photoelectric heating

hv:

W:

Y:



Hollenbach & Tielens, 1999, Rev. Mod. Phys., Vol. 71

"A far-ultraviolet photon absorbed by a dust grain creates a photoelectron which diffuses through the grain until it loses all its excess energy due to collisions with the matrix or finds the surface and escapes. For PAHs, the diffusion plays no role."

- photon energy work function of the grain Coulomp potential of the grain
 - ionization potential of the PAH
- yield, i.e. probability that the photon escapes (~ 0.1 for large grains)
- efficiency, i.e. fraction of escaping photon times fraction of energy carried away

Photoelectric heating



Photoelectric heating

$$n\Gamma_{\rm pe} = 10^{-24} \epsilon n G_0 \,{\rm erg} \,{\rm cm}^{-3} \,{\rm s}^{-1}.$$

$$\epsilon = \frac{4.87 \times 10^{-2}}{1 + 4 \times 10^{-3} \gamma^{0.73}} + \frac{3.65 \times 10^{-2} (T/10^4)^{0.7}}{1 + 2 \times 10^{-4} \gamma}$$

see also: Bakes & Tielens 1994 Weingartner & Draine 2001

 $\gamma = G_0 T^{1/2} / n_e$ charging parameter: photo-ionization over recombination rate

The work function of grains is ~ 5-7 eV. 50% of the PE heating is contributed by grains < 15 Å. PAH's heat more efficiently than large grains.

H₂ pumping



- line absorption of FUV photons pumps electronically excited state (Lyman, Werner bands)
 - 10-15 % fluoresce back to vib. continuum of the ground el. state \rightarrow photo-dissociation
 - 85-90 % fall back to bound vib. states of the el. ground state
 - $\rightarrow E_{vib}$ ~ 2 eV available for heating
- efficient at high densities

$$n\Gamma_{\rm H_2} \simeq 2.9 \times 10^{-11} nn_{\rm H} k_{\rm d} \left[1 + \left(\frac{n_{\rm cr}}{n}\right) + \frac{4.4 \times 10^2 G_0}{n T^{1/2} \exp[-1000/T]} \right]^{-1} \operatorname{erg} \, \mathrm{cm}^{-3} \, \mathrm{s}^{-1}$$



- H₂ forms on dust surfaces
- binding energy of $H_2 \sim 4.5 \text{ eV}$
 - newly formed H₂ molecules are released into the gas-phase and carry away part of the binding energy as kinetic and internal energy
 → heating via collisions

$$\Gamma_{\rm H_2 \ form} = 2.4 \times 10^{-12} R_{\rm H_2 \ form} n_{\rm H} \,\rm erg \, \rm cm^{-3} \, \rm s^{-1}$$

R_{H2form}: H₂ formation rate



formation efficiency

- H-binding to the grain surface determines its mobility and resistance against thermal desorption
 - weak binding (physisorption), T<50-80K
 - strong binding (chemisorption), T<~500-800 K

Chemisorption leads to efficient H_2 formation at high temperatures



Chemisorption leads to efficient H_2 formation at high temperatures



More efficient H2 formation leads to stronger gas heating.



More efficient H2 formation leads to stronger gas heating.

Röllig et al. 2013



Dust content & physics influences high-J CO emission

Röllig et al. 2013

H₂ dissociation heating

- When H₂ is excited into the Lyman and Werner bands, there is about 10% chance that it will decay into the vibrational continuum, thus dissociating the molecule.
- Each of the H atoms created this way carries approximately 0.4 eV.

$$\Gamma_{\text{H}_2 \text{ diss}} = 6.4 \times 10^{-13} n (\text{H}_2) R_{\text{H}_2 \text{ diss}} \text{ erg cm}^{-3} \text{ s}^{-1}$$

Gas-grain collisions

If T_{gas} ≠ T_{dust} collisions between the two components will transport energy from the hotter to the cooler.

$$\Lambda_{g\text{-}gr} = n_{gr} n_{H} \sigma_{gr} \left(\frac{8kT_{g}}{\pi m_{H}}\right)^{1/2} \bar{\alpha}_{T} (2kT_{g} - 2kT_{gr})$$

Burke & Hollenbach 1983

 α_{T} : accomodation factor, i.e. average energy transfer fraction (=1 if incoming particle fully thermalizes with the surface)



Gas-grain collisions

accomodation factor



Carbon ionization

$$\Gamma_{\rm C \ ion} = 1.7 \times 10^{-12} R_{\rm C \ ion} n({\rm C}) \,{\rm erg}\,{\rm cm}^{-3}\,{\rm s}^{-1}$$

 Photo-ionization of atomic carbon releases a hot electron (~ 1 eV), heating the gas via collisions.

R_{Cion}: carbon ionization rate

Cosmic ray heating

- Cosmic rays (e.g.: high energy 2-10 MeV) ionize the gas (H₂, He, HD) and inject hot e⁻ into the gas.
- The efficiency depends on the gas composition, density and ionization degree. Ionization of H and H2 contributes 3.5 and 8 eV respectively.
- Cosmic rays can penetrate much deeper into a molecular cloud (~ A_v=100) than UV photons (A_v<10). CR's are the dominant heating term at high optical depths.

$$\Gamma_{\rm CR} = \zeta_{\rm CR} \left(5.5 \times 10^{-12} n_{\rm H} + 2.5 \times 10^{-11} n_{\rm H_2} \right) \qquad \xi_{\rm CR} \simeq 3 \times 10^{-16} \, {\rm s}^{-1}$$

Radiative line cooling

- When a transition of a species is excited collisionally and decays radiatively, the transition energy is carried away by photons and the gas is cooled.
- Coolant conditions:
 - abundant
 - collisionally excitable energy levels given ISM conditions
 - rapid decay times (large A_{ij})
- Good coolants: C⁺, O, C, CO, H₂O

Radiative line cooling

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/ in	300	-		_ 10	- QN(up) (K1	QN(low) J <u>K K1</u>	Freq (GHz)	A(U-L)	B(L–U)	Log(Tau) relative
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	200 -	- -		_ 08	06 07 08 09		05 06 07 08	691.473 806.652 921.800	2.23E-05 3.58E-05 5.38E-05 7.71E-05	5.40E+06 5.33E+06 5.28E+06 5.24E+06	0.94 0.82 0.63 0.40
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CO

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- Coolant conditions:
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Fine-Structure Atomic Cooling Parameters								
Species (0, 1, 2) ^a	$\frac{E_{ij}}{k}$ (K) ^b	λ _μ °	$n_{\rm cr}^e ({\rm cm}^{-3})^d$	$n_{\rm er}^{\rm H} ({\rm cm}^{-3})^{\rm d}$	$A_{ij} (\mathrm{s}^{-1})^{\mathrm{e}}$	$\gamma_{ij}^{e} (cm^{-3} s^{-1})^{f}$	$\gamma_{ij}^{H} (cm^3 s^{-1})^{f}$	$N_{\tau} ({\rm cm}^{-2})^{g}$
$C_1({}^3P_0, {}^3P_1, {}^3P_2)$	2.4(1) 6.3(1) 3.9(1)	609.2 229.9 369.0	3.9(0)T ₂ ^{-0.13} 1.3(1)	$\frac{1.6(2)T_2^{-0.34}}{7.0(2)T_2^{-0.26}}$	7.9(-8) 2.0(-14) 2.7(-7)	3.0(-9) 5.0(-9) 1.5(-8)	$\begin{array}{c} 1.6(-10)T_2^{0.14} \\ 9.2(-11)T_2^{5.26} \\ 2.9(-10)T_2^{0.26} \end{array}$	2.3(20) 9.8(27) 5.3(20)
$C \pi ({}^{2}P_{1/2}, {}^{2}P_{3/2})$	9.2(1)	157.7	8.7(0)T ^{0.50} ₂	$3.0(2)T_2^{-0.07}$	2.4(-6)	$2.8(-7)T_2^{-0.5}$	$8.0(-10)T_2^{0.07}$	6.5(20)
$Cl_1({}^2P_{3/2}, {}^2P_{1/2})$	1.3(3)	11.4	2.6(5)	$1.4(7)T_2^{-0.17}$	1.2(-2)	4.7(-8)	$8.3(-10)T_2^{0.17}$	1.1(24)
$\operatorname{Cln}({}^{3}P_{2}, {}^{3}P_{1}, {}^{3}P_{0})$	1.0(3) 1.4(3) 4.3(2)	14.4 10.0 33.4	$1.4(4)T_2^{0.45}$ $1.6(3)T_2^{0.50}$	5.4(6) 8.1(5)	7.5(-3) 4.8(-7) 1.4(-3)	$5.3(-7)T_2^{-0.5}$ $5.3(-7)T_2^{-0.5}$ $3.2(-7)T_2^{-0.5}$	1.4(-9) 1.1(-9) 6.3(-10)	7.5(23) 1.0(29) 5.7(23)
Fei(⁵ D ₄ , ⁵ D ₃ , ⁵ D ₂)	6.0(2) 1.0(3) 4.2(2)	24.0 14.2 34.2	$2.1(4)T_2^{-0.13}$ 7.5(3)	$3.1(6)T_2^{-0.28}$ $1.3(6)T_2^{-0.17}$	2.5(-3) 1.0(-9) 1.6(3)	1.2(-7) 1.2(-7) 9.3(-8)	$\begin{array}{c} 8.0(-10)T_2^{0.17} \\ 6.9(-10)T_2^{0.17} \\ 5.3(-10)T_2^{1.17} \end{array}$	6.6(21) 9.3(26) 3.7(21)
Fеп (⁶ D _{9/2} , ⁶ D _{7/2} , ⁶ D _{5/2})	5.6(2) 9.6(2) 4.1(2)	26.0 15.0 35.4	$1.2(3)T_2^{0.41}$ $6.0(2)T_2^{0.50}$	$2.2(6)T_2^{-0.09}$ 1.5(6)	2.1(-3) 1.5(-9) 1.6(-3)	$\frac{1.8(-6)T_2^{-0.5}}{1.8(-6)T_2^{-0.5}} \\ 8.7(-7)T_2^{-0.5}$	9.5(-10) 5.7(-10) 4.7(-10)	6.0(21) 5.9(28) 3.3(21)
Ne II $({}^{2}P_{3/2}, {}^{2}P_{1/2})$	1.1(3)	12.8	5.4(4)T ^{0.50} ₂	6.6(6)	8.6(-3)	$1.6(-7)T_2^{-0.5}$	1.3(-9)	1.9(22)
$Ni1({}^{3}F_{4}, {}^{3}F_{3}, {}^{3}F_{2})$	1.9(3) 3.2(3) 1.3(3)	7.5 4.5 11.3	$5.2(5)T_2^{-0.06}$ 1.2(5)	$7.8(7)T_2^{-0.22}$ $2.0(7)T_2^{0.17}$	6.2(-2) 3.6(-9) 2.5(-2)	1.2(-7) 1.2(-7) 9.3(-8)	$\begin{array}{c} 8.0(-10)T_2^{0.17} \\ 6.9(-10)T_2^{0.17} \\ 5.3(-10)T_2^{0.17} \end{array}$	1.1(23) 1.3(31) 8.9(22)
Ni II $({}^{2}D_{5/2}, {}^{2}D_{3/2})$	2.2(3)	6.6	5.0(4)T20.50	50(7)	5.5(-2)	$1.1(-6)T_2^{-0.5}$	1.1(-9)	2.2(23)
$O_1({}^3P_2, {}^3P_1, {}^3P_0)$	2.3(2) 3.3(2) 9.8(1)	63.1 44.2 145.6	$6.3(3)T_2^{-0.03}$ 8.9(2)	$\begin{array}{c} 8.5(5)T_2^{-0.69} \\ 1.1(5)T_2^{-0.57} \end{array}$	9.0(-5) 1.0(-10) 1.7(-5)	1.4(-8) 1.4(-8) 5.0(-9)	$9.2(-11)T_2^{0.67} 4.3(-11)T_2^{0.80} 1.1(-10)T_2^{0.44}$	4.9(20) 3.8(27) 3.7(20)
$S : ({}^{3}P_{2}, {}^{3}P_{1}, {}^{3}P_{0})$	5.7(2) 8.2(2) 2.5(2)	25.2 17.4 56.6	$4.2(4)T_2^{-0.03}$ 6.7(3)	$\frac{1.8(6)T_2^{-0.22}}{2.7(5)T_2^{-0.17}}$	1.4(-3) 7.1(-8) 3.0(-4)	3.3(-8) 3.3(-8) 1.2(-8)	$7.5(-10)T_2^{0.17}7.1(-10)T_2^{0.17}4.2(-10)T_2^{0.17}$	2.0(22) 3.7(27) 1.5(22)
Sit $({}^{3}P_{0}, {}^{3}P_{1}, {}^{3}P_{2})$	1.1(2) 3.2(2) 2.1(2)	129.6 44.8 68.4	$7.2(2)T_2^{-0.50}$ 1.4(3)	$\begin{array}{c} 1.9(4)T_2^{-0.47} \\ 6.3(4)T_2^{-0.17} \\ \end{array}$	8.4(-6) 2.4(-10) 4.2(-5)	7.2(-9) 7.2(-9) 2.2(-8)	$3.5(-10)T_2^{-0.03}$ $1.7(-10)T_2^{0.17}$ $5.0(-10)T_2^{0.17}$	2.3(21) 2.0(27) 5.6(21)
$Si u ({}^{2}P_{12}, {}^{2}P_{32})$	4.1(2)	34.8	1.2(2)T ^{0.50} ₂	3.2(5)	2.1(-4)	$1.7(-6)T_2^{-0.5}$	$8.0(-10)T_2^{-0.07}$	7.1(21)

^a The levels are arranged as follows: 0 = ground state, 1 = first excited state, and 2 = second excited state.

^b For three-level systems, the energies listed are E10, E20, and E21, respectively.

⁶ The wavelength in microns; note that the 2→0 transition is generally forbidden.

^d The critical densities (see text) are listed to achieve LTE in levels 1 and 2, respectively, $T_2 = T/100$ K. The power law fits for the three level systems are accurate to 30% in the temperature range 30 K < T < 3000 K.

^e The spontaneous transition rates listed in order A₁₀, A₂₀, and A₂₁. These are taken from Aller (1984), Garstang 1958, 1962, 1964, 1968; Grevesse, Nussbaumer, and Swings 1971; and Wiese et al. 1966, 1969.

^f The rate coefficients for collisional deexcitation are listed in the same order. They are calculated from formulae given by Bahcall and Wolf 1968 with the exceptions C 1 and O 1 (Launay and Roueff 1977a), C II (Launay and Roueff 1977b), Fe II (Aannestad 1973), Ne II (Osterbrock 1974). Proton rates are substituted for electron rates for neutral target atoms.

* N_x is the column density of hydrogen nuclei which provide unit optical depth at line center, assuming solar abundances of the species in the lower state of the transition.

Hollenbach & Mckee, 1989, ApJ 342, 306

Radiative line cooling

$$\Lambda_X(\nu_{ij}) = n_i A_{ij} h \nu_{ij} \beta_{\text{esc}}(\tau_{ij}) \frac{S(\nu_{ij}) - P(\nu_{ij})}{S(\nu_{ij})}$$

$$S(v_{ij}) = \frac{2hv_{ij}^3}{c^2} \left(\frac{g_i n_j}{g_j n_i} - 1\right)^{-1}$$

$$\frac{\mathrm{d}n_i}{\mathrm{d}t} = \sum_{j \neq i} n_j R_{j \to i} - n_i \sum_{j \neq i} R_{i \to j} = 0$$

$$P(v_{ij}) = B_{v_{ij}}(T_{\text{CMB}}) + \tau_{\text{dust}}B_{v_{ij}}(T_0)$$

- radiative cooling rate due to transition
 i→j of a species *x*
- local source function

- level populations from the equations of statistical equilibrium
- background radiation

Radiative line cooling











H₂ excitation



H₂ excitation



higher H₂ transition (J_{up}>3) can not easily be reproduced by PDR models

CO Dissociation



- CO dissociation occurs via line absorption!
- Absorbed photons excite *predissociated* electronic states that can decay into unbound continuum of the ground elect. state radiationless.
- More than 30 absorption bands in the range 913 Å $\leq \lambda \leq$ 1077 Å
- Line absorption leads to optical thickness effects (self-shielding)

Warin et al. 1996

CO Dissociation



Warin et al. 1996

Chemistry

The carbon roadmap

- Like any roadmap, this network describes how to get from A to B.
- Like on any roadmap, some paths are quick some are slow.
- Unlike any normal roadmap some slow paths may become very quick under certain conditions





Example: PDR high FUV intensity heats the gas at the surface \rightarrow some slow routes become quick $C^+ + H_2 \rightarrow CH^+ + H$ $C^+ + H_2^+ \rightarrow CH^+ + H$

endothermic reactions become possible activation energy barriers become surmountable



Example: Dark Cloud cold and dense: T=10 K, n=10⁴-10⁵ cm⁻³ carbon locked in CO He + c.r \rightarrow He⁺ + e $He^+ + CO \rightarrow C^+ + O + He$ FUV fully absorbed some roads vanish some roads become slow e.g. reactions with ebut: $CH_5^+ + CO \rightarrow CH_4 + HCO^+$



Looks 'simple', but:

CH⁺ a factor 100 too low

H₂ formation not fully understood



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13.02.2014

a 16 16











- H₂ photodissociation is a line absorption process. Once the absorption lines become optically thick, photodissociation becomes inefficient
- Density and UV field strength determine the depth of the H-H₂ transition zone



- CO photodissociation is shielded by
 - itself (self-shielding)
 - CO isotopologues (mutual shielding)
 - overlapping H2 lines
 - dust attenuation
- CO photodissociation becomes inefficient for N_{CO} >10¹⁶ cm⁻²



 "Standard" models show a good H2-HF correlation (agreement with empirical findings)



• H₂-CH correlation changes from diffuse to denser clouds



Röllig & Ossenkopf 2013, A&A 550, A56



- OH appears to be a reasonable PDR interface tracer
- column densities not well modelled



XDR or PDR? (Spaans & Meijerink 2007, ApJ 664, L23)

				TABLE	1							
	COLUMN DENSITIES AND COLUMN DENSITY RATIOS											
N _H	<i>N</i> (CO ⁺)	N(HOC ⁺)	<i>N</i> (HCO ⁺)	N(CN)	N(HCN)	CO ⁺ /HCO ⁺	HCO ⁺ /HOC ⁺	CN/HCN				
XDR: $n = 10^5 \text{ cm}^{-3}$ and $F_x = 5.1 \text{ ergs s}^{-1} \text{ cm}^{-2}$												
1.0E22	3.0E12	3.3E12	4.3E13	1.1E15	6.0E12	0.07	13.2	181				
2.0E22	4.8E12	5.0E12	1.6E14	2.7E15	2.8E13	0.03	31.5	95.4				
3.0E22	5.7E12	5.9E12	2.7E14	4.7E15	5.9E13	0.02	46.4	78.9				
XDR: $n = 10^{3.5} \text{ cm}^{-3}$ and $F_x = 1.6 \text{ ergs s}^{-1} \text{ cm}^{-2}$												
3.0E22	1.2E12	5.7E11	1.5E12	5.2E13	3.2E10	0.8	2.6	1.6E3				
6.0E22	8.3E12	6.9E12	3.7E13	5.1E14	9.4E11	0.2	5.4	543				
9.1E22	1.8E13	1.5E13	1.3E14	1.5E15	3.8E12	0.14	8.5	400				
PDR: $n = 10^5 \text{ cm}^{-3}$, $G_0 = 10^{35}$, and $\zeta = 5 \times 10^{15} \text{ s}^{-1}$												
1.0E22	1.6E10	1.0E10	2.8E14	2.3E15	3.5E14	5.6E-5	2.8E4	6.6				
2.0E22	1.7E10	1.5E10	7.8E14	4.5E15	9.5E14	2.2E-5	5.2E4	4.7				
3.0E22	1.9E10	2.0E10	1.3E15	6.7E15	1.6E15	1.4E-5	6.5E4	4.3				





Credit: Slide by A. Fuente

XDR vs. PDR



Spaans & Meijerink 2008

PDR Emission



PDR Emission



PDR diagnostics



$\begin{aligned} & \mathsf{Y}_{[\mathsf{CII]}} = \mathsf{I}_{[\mathsf{CII]}} / \mathsf{I}_{\mathsf{FIR}} \\ & \mathsf{Y}_{\mathsf{CO}} = \mathsf{I}_{\mathsf{CO}} / \mathsf{I}_{\mathsf{FIR}} \end{aligned}$

Stacey et al. 1991

SOFIA Winter School 2014 - Cologne

PDR diagnostic model diagrams



- Absolute intensities always involve an (unknown) filling factor
- Lorenzetti et al (1999) used the [OI]_{63µm}/[CII]_{157µm} and [OI]_{63µm}/[OI]_{145µm} intensity ratios to derive the physical conditions of the PDRs associated with Herbig Ae/Be stars based on ISO data.

PDR diagnostic model diagrams

PDR diagmostic diagrams are useful to derive global properties. If the main heating mechanism is the photoelectric effect, heating efficiency depends on the grain charge which is itself governed by the paramter $G_0 T^{1/2} / n_e$.



Figure 9.9 A diagnostic diagram for PDRs based on the observed intensity ratio of the [CII] 158 μ m and [OI] 63 μ m lines and the overall cooling efficiency. The lines present the results of detailed model calculations for different densities and incident FUV fields. Figure kindly provided by M. J. Kaufman; derived from the models described in M. J. Kaufman, M. G. Wolfire, D. Hollenbach, and M.L. Luhman, 1999, *Ap. J.*, 527, p. 795.



Gas heating efficiency

Since the [CII] 158 µm and [OI 63 µm lines have different critical densities, their intensity ratio is a good measure of the density.

Diagnostic Plots





[CII] contribution from HII regions

Teff= 42000 K



- C⁺ is also present in the ionized gas
- When observing a PDR you always observe the neighbouring HII region
- [CII] emission is partly produced in the HII region.

[CII] contribution from HII regions

Teff= 42000 K





Bernard-Salas et al. 2012

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