

GMC Microphysics

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AST 542
October 2, 2012

Outline

Introduction to PDRs

Overview

PDR Chemistry

H₂ Formation and Dissociation

CO formation and dissociation

Grain Chemistry

Heating and Cooling

Heating Processes

Cooling Processes

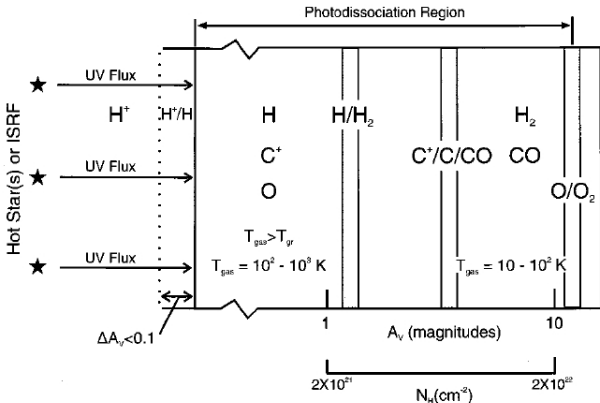
Simulations

Conclusions

Overview

- ▶ A photodissociation region (PDR) is the interface between an HII Region and a molecular cloud
- ▶ It is marked by a photodissociation surface— a region where the hydrogen is half atomic and half molecular
- ▶ Nearly all of the atomic gas and most of the molecular gas in a galaxy can be found in a PDR

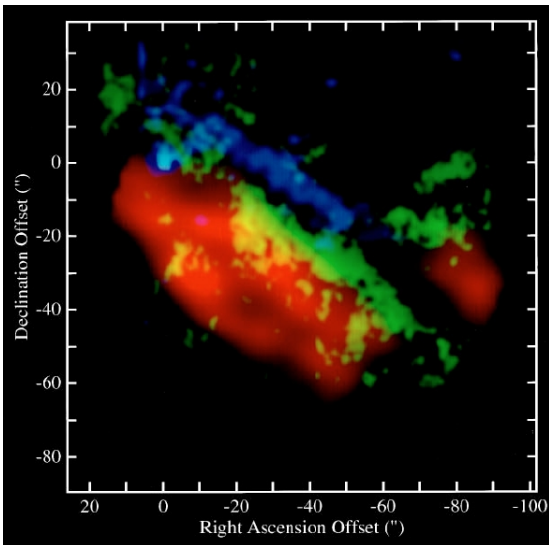
Structure



Tielens and Hollenbach 1999

- ▶ We will discuss each of the zones in a PDR in detail

Observation



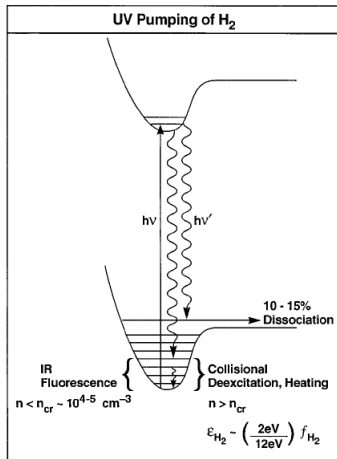
Tielens et al 1993

H₂ Formation and Dissociation

- ▶ H₂ is by far the most common molecule in PDRs (factor 10⁴ more abundant than CO)
- ▶ Most H₂ forms on the surfaces of dust grains

H₂ Formation and Dissociation

- ▶ Upon absorption of a FUV photon, H₂ has a $\sim 10 - 15\%$ chance of dissociating
- ▶ Otherwise, H₂ will remain in a vibrationally excited state. Collisional de-excitation from this state can heat the gas

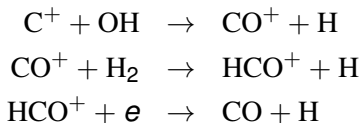


Self-Shielding

- ▶ Because the H_2 density is so high, FUV lines can become optically thick
- ▶ This creates a sharp transition between HI and H_2
- ▶ The location of this transition is set both by self-shielding (high density / low radiation regime) and by dust opacity (low density / high radiation regime)

CO Formation and Dissociation

- ▶ C^+ and C are balanced by photoionization and radiative recombination
- ▶ CO formed through burning neutral radicals like CH and CH_2
- ▶ Alternatively:



- ▶ CO is slow to form because its reactants have relatively low abundance
- ▶ CO is not significantly shelf-shielded due to low abundance
- ▶ Thus, CO exists primarily deep within a cloud, and the transition to CO is set by dust extinction

Dust

- ▶ Silicate and carbonaceous grains provide the dominant source of opacity
- ▶ Dust receives $10^2 - 10^3$ more heating than the gas, but maintains lower temperature by effective cooling
- ▶ Greatly affect heating/cooling balance via IR radiation
- ▶ Also important for catalyzing H_2 formation

PAHs

- ▶ Polycyclic aromatic hydrocarbons (PAHs) are large carbon molecules that give rise to distinctive IR features
- ▶ Typical size: 50 C atoms, giving a PAH abundance relative to H of $\sim 10^{-7}$
- ▶ Important for photoelectric heating

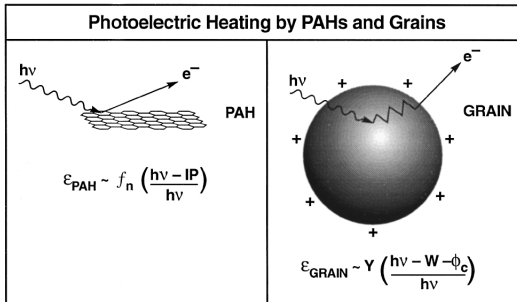
Heating and Cooling

- ▶ Heating
 - ▶ Photoelectric Heating
 - ▶ Collisional De-excitation
 - ▶ Cosmic Ray Heating
- ▶ Cooling
 - ▶ Atomic Line Emission
 - ▶ Molecular Line Emission
 - ▶ Collisional Excitation
 - ▶ Grain Cooling

Photoelectric Heating

- ▶ UV photons can liberate electrons from PAHs
- ▶ An ejected photoelectron can then heat the gas
- ▶ Photoelectric heating is dominated by the smallest grains
- ▶ 0.1 – 1% of the UV intensity goes into photoelectrons ejected by PAHs

Photoelectric Heating Schematic



Tielens and Hollenbach 1999

- ▶ Limiting factor for high-efficiency small grains is that some may have an ionization potential $> 13.6 \text{ eV}$
- ▶ Efficiency drops as PAHs become more charged

Collisional De-excitation

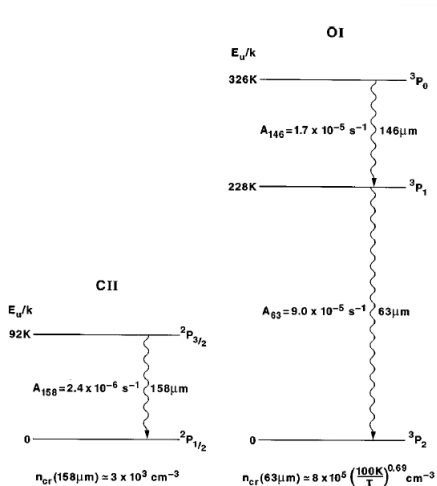
- ▶ Recall that H_2 molecules may absorb a photon, then decay radiatively to a vibrationally excited state
- ▶ At high densities, these molecules may be de-excited via collisions with atomic H, thereby heating the gas
- ▶ A vibrationally excited H_2 molecule has ~ 2 eV of vibrational energy

Cosmic Ray Heating

- ▶ At high densities, cosmic ray ionization of molecules becomes important
- ▶ Standard H₂ cosmic ray ionization rate of 3×10^{-17} molecules per second
- ▶ Important for ionizing in regions where UV does not penetrate

Atomic Line Emission

- ▶ Infrared fine structure lines, notably [CII] 158 μm and [OI] 63 μm , 146 μm
- ▶ The [CII] fine structure line often dominated cooling in the ISM of a galaxy

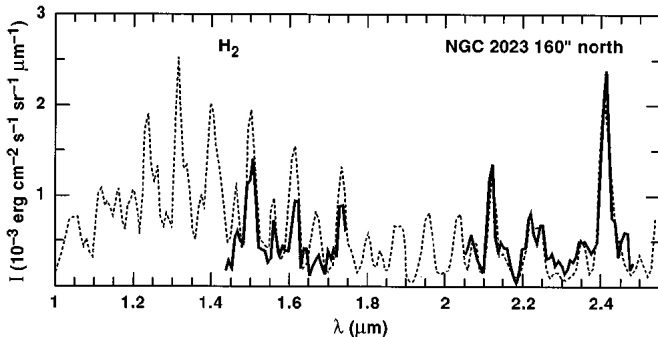


Atomic Line Emission

- ▶ [CII] and [OI] lines are good for determining density and temperature since their range of critical densities ($3 \times 10^3 - 3 \times 10^5 \text{cm}^{-3}$) and excitation temperatures (100 – 300K) span the range of conditions found in PDRs
- ▶ Ratio of the cooling rate to FIR dust emission yields the photoelectric heating efficiency

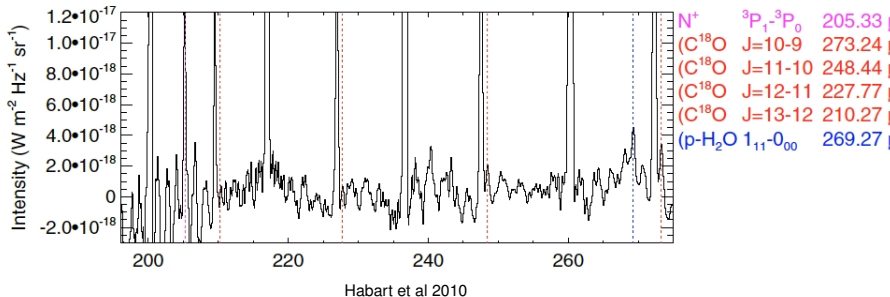
Molecular Line Emission

- ▶ Ro-vibrational emission from H₂



- ▶ UV-pumped H₂ decays via electric quadrupole transitions, emitting in the red and NIR

Molecular Line Emission



- ▶ The dipole moment of CO allows it to be an effective radiator

CO to H₂ Relation

- ▶ The strength in the CO 1-0 line has been observed to correlate well with the mass of H₂

$$X_{CO} \equiv N(\text{H}_2) / \int T_A dv$$

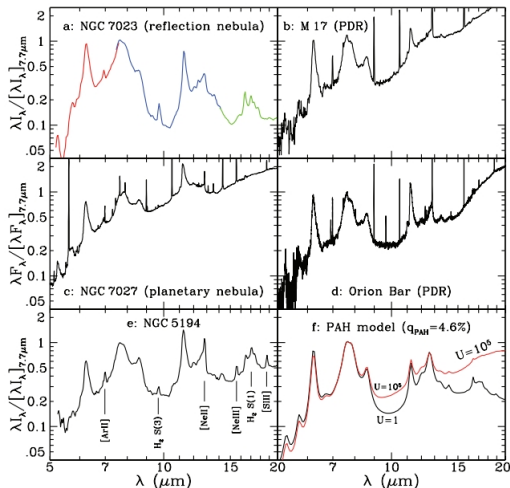
- ▶ In “dark molecular gas” (Wolfire 2010), the hydrogen is in molecular form but the CO is not
- ▶ ~30% of the molecular cloud mass may be in such gas

Collisional Excitation

- ▶ Collisional excitation of atoms, molecules, and ions by electrons, H, or H₂ followed by radiative decay cools the gas

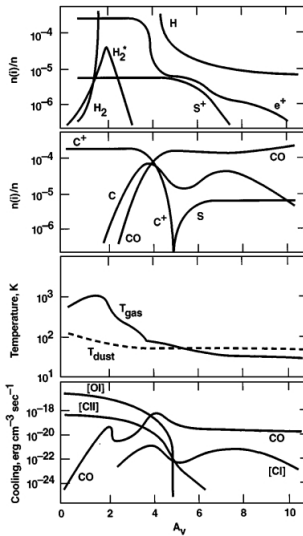
Grain Cooling

- ▶ Grains absorb UV radiation and re-radiate in the IR
- ▶ Collisions with grains, which are typically cooler than the gas, can also lead to net cooling

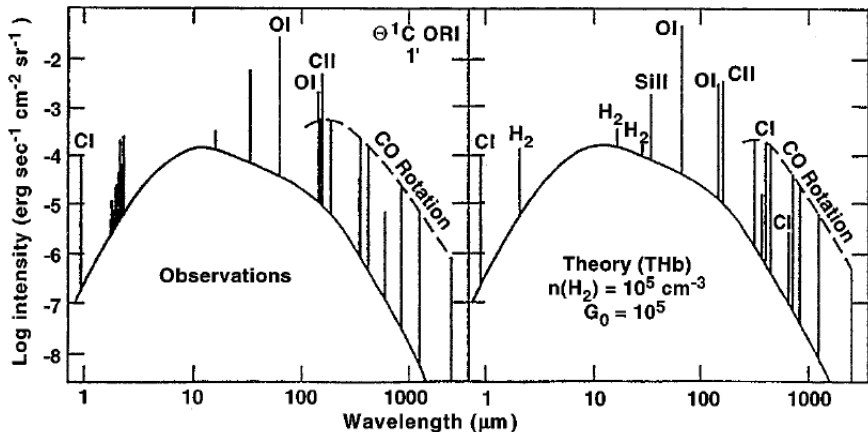


Summary

- ▶ We can now understand the detailed structure and spectrum of a PDR



Summary



Tielens and Hollenbach 1999

Simulations

Simulations

Simulations

- ▶ Simulations of PDRs can be difficult
 - ▶ Reaction rates can span many orders of magnitude—timestep needs to be quite small
 - ▶ Solving for abundance of N species implicitly goes as $O(N^3)$
 - ▶ 3D problem with turbulence, magnetic fields...
- ▶ Some common simplifications are made

Gas Clumpiness

- ▶ Molecular gas will be inherently clumpy, but can it be modeled as a constant-density medium?
- ▶ Levier et al 2012 compared clumpy vs constant density models of PDRs and found constant density models underpredicted chemical abundances by a factor of 2 – 4
- ▶ Also found 35 – 40% dark molecular gas

Simulations and XCO

- ▶ Glover and Clark 2012 studied a range of PDR simulations, from relatively simple to quite complex
- ▶ Varied primarily in complexity of chemical reactions / species considered
- ▶ Fairly robust agreement in value of X_{CO} , lending credence to universality of the relation that is relatively insensitive to chemistry
- ▶ However, CO *distribution* varied considerably among models

Simulations and XCO

Table 2. Computational performance of the various approaches.

Method	Approximate runtime (CPU hours)	
	Run 1	Run 2
G10g	1190	1360
G10ng	880	1240
NL97	110	140
NL99	310	460
KC08e	100	130
KC08n	120	150

Glover and Clark 2012

Table 4. Comparison of the CO-to-H₂ conversion factor X_{CO} , at the end of the runs.

Method	X_{CO} [$10^{20} \text{ cm}^{-2} (\text{K km s}^{-1})^{-1}$]	
	Run 1	Run 2
G10g	2.67	1.30
G10ng	2.01	1.23
NL97	0.57	0.90
NL99	1.47	1.17
KC08e	0.50	0.89
KC08n	0.49	0.87

Glover and Clark 2012

Summary

- ▶ PDRs are a site of rich interstellar chemistry that has dramatic effects on gas structure, temperature, etc
- ▶ Simulations of PDRs are difficult but have been successful in reproducing key observables