Photodissociation Regions

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1. Introduction

The opening of the infrared and microwave parts of the spectrum has enabled us to probe processes that cannot be observed directly in the optical. We have already encountered one such example, namely the thermal emission from dust grains. Following our discussion of molecular structure, we now have the tools to examine other regions best studied in the infrared: the **molecular clouds** in which stars form, and the **photodissociation regions** (PDRs) that separate the bulk of the cloud from the H II regions ionized by young stars. As a matter of principle, the PDR is actually an extension of the H II region, a region where the gas is mostly neutral but with an extensive network of chemical reactions driven by radiation at $h\nu$<13.6 eV that can penetrate through atomic gas. Beyond the PDR lies dense, cold molecular material, where the column of dust essentially extinguishes ultraviolet light from stars. Cosmic rays penetrating this region provide a small amount of heat and ionization, enabling a rich sequence of chemical reactions to occur.

We will treat the PDR in these notes as a constant-*pressure* rather than constant-density environment. This is a better approximation in the case of narrow regions with subsonic motions and large temperature gradients.

The principal reference for these notes is Tielens, Ch. 9. In particular, our discussion of diagnostics follows Tielens §9.7.

2. The Life Cycle of H_2

We begin our discussion by investigating the formation and destruction of H_2 molecules.

A. FORMATION OF H_2

Our discussion of molecular gas begins with investigation of how atoms can form molecules. One's first thought would be that H atoms can simply combine to form H_2:

$$2\mathrm{H} \rightarrow \mathrm{H}_2 + \gamma.$$

In fact this process is forbidden because there is no dipole moment. More precisely, one may view the two H atoms as forming an unbound vibrational state of H_2. The electrons for the initial atoms may form a spin singlet (term: ${}^1\Sigma_g^+$) or a spin triplet (term: ${}^3\Sigma_u^+$); neither has an allowed decay to the ground state of H_2 (${}^1\Sigma_g^+$).

A second possibility would be to use a 3-body reaction

$$3\mathrm{H} \rightarrow \mathrm{H}_2 + \mathrm{H}$$

or a catalyst:

$$\mathrm{H} + e^- \rightarrow \mathrm{H}^- + \gamma,$$
$$\mathrm{H}^- + \mathrm{H} \rightarrow \mathrm{H}_2 + e^-.$$

These reactions are slow: the first requires extremely high densities since it requires the simultaneous collision of 3 atoms, and the second requires ionization (which is low in the cold regions most likely to form molecules) and has a small rate coefficient at low temperatures (selection rules require the initial electron to have odd angular momentum, which implies an angular momentum barrier). These reactions may be important in primordial galaxies, where there are no alternative pathways to form H_2, but in the modern ISM H_2 can form efficiently on dust grains.

The formation of H_2 on dust begins with a hydrogen atom being adsorbed onto its surface: the atom collides with the surface, and enough energy is dumped into vibrational modes of the grain that the atom can stick (forming a van der Waals bond). These H atoms then quantum-mechanically tunnel among the possible adsorption sites on the grain surface, until they react to form H_2. The bond energy of H_2 (4.5 eV) is sufficient to detach the molecule from the grain and release it into the gas phase.

The rate coefficient for the catalyzed reaction

$$2\mathrm{H} \xrightarrow{\text{dust}} \mathrm{H}_2$$

can be computed assuming that all hydrogen atoms colliding with a dust grain react. The coefficient (units: cm^3/s) is

$$k = \frac{1}{2}\int \pi a^2 v_{\rm H} \frac{1}{n_{\rm H}} \frac{dn_{\rm gr}}{da} da,$$

where we have used the mean velocity $v_{\rm H}$ of the hydrogen atoms, which is proportional to $T^{1/2}$. If all grains had the same size a, then we could write this integral in terms of the grain volume:

$$k = \frac{1}{2}\pi a^2 v_{\rm H} \frac{n_{\rm gr}}{n_{\rm H}} = \frac{1}{2}\pi a^2 v_{\rm H} \frac{V_{\rm gr}}{\frac{4}{3}\pi a^3} = \frac{3}{8}\frac{v_{\rm H}}{a} V_{\rm gr};$$

here $V_{\rm gr}$ is the grain volume per H atom. Since the grain mass per H atom (determined by the abundance of the depleted metals) is $\sim 0.005 m_{\rm H}$, we have $V_{\rm gr} \sim 3\times10^{-26}$ cm^3. The typical size is $a \sim 0.2$ μm, and the mean velocity is $5\times10^5 T_3^{1/2}$ cm/s. Thus we find

$$k \sim 3\times10^{-16} T_3^{1/2}\ {\rm cm^3/s}.$$

This simplistic argument appears to be roughly correct, although the actual rate derived from observations of diffuse clouds is a factor of a few lower.

B. H_2 PHOTODISSOCIATION AND FLUORESCENCE

The destruction of H_2 is usually driven by UV radiation, since at molecular cloud or even PDR temperatures collisional dissociation is inefficient. One might at first imagine that the reaction:

$$\mathrm{H_2} + \gamma \rightarrow 2\mathrm{H}$$

is possible; however as discussed earlier there is no dipole moment. One might then imagine direct photoionization:

$$\mathrm{H_2} + \gamma \rightarrow \mathrm{H_2^+} + e^-,$$

but the photon energy required is at least 15 eV and hence cannot occur in regions shielded by neutral hydrogen.

In fact, the principal interaction of UV photons with H_2 involves excited electronic states. Recall that the ground electronic state of H_2, $X^1\Sigma_g^+$, consists of both electrons in the lowest σ_g orbital. The following are then possible:

- Absorption of a photon with electric field *parallel* to the internuclear axis can excite one electron into the lowest σ_u orbital. This puts the molecule into the $B^1\Sigma_u^+$ electronic state. The associated absorption lines are called the **Lyman band** and have a minimum energy of 11.2 eV.

- Absorption of a photon with electric field *perpendicular* to the internuclear axis can excite one electron into the lowest π_u orbital. This puts the molecule into the $C^1\Pi_u$ electronic state. The associated absorption lines are called the **Werner band** and have a minimum energy of 12.3 eV.

The electronically excited H_2 molecules will decay back to the $X^1\Sigma_g^+$ state, and in doing so emit UV radiation. There may also be IR radiation since the molecule generally does not decay back into the ground rotation-vibration state. This radiation is known as **H_2 fluorescence**.

The H_2 molecule may also decay back into an unbound vibrational state. In such a case it is destroyed. The net reaction is:

$$\mathrm{H}_2(X^1\Sigma_g^+) + \gamma \rightarrow \mathrm{H}_2(B^1\Sigma_u^+ \text{ or } C^1\Pi_u) \rightarrow 2\mathrm{H}(1\mathrm{s}_{1/2}) + \gamma.$$

The rate of this reaction is determined by the frequency-averaged cross section of the Lyman and Werner lines, the probability p to dissociate the molecule, and the intensity of the radiation field. This is $k_{\mathrm{UV}} \sim 4\times10^{-11} G_0\ \mathrm{s}^{-1}$.

In a PDR with $G_0 \sim 10^4$, an H_2 molecule may "live" for only a month before being destroyed. The abundance of H_2 relative to H^0 is determined by the rate at which H_2 can be re-formed:

$$\frac{n(\mathrm{H}_2)}{[n(\mathrm{H}^0)]^2} = \frac{k}{k_{\mathrm{UV}}}.$$

Thus we see that the radiation intensity G_0 (denominator), and the temperature (numerator), as well as the density, determine the balance of atomic versus molecular hydrogen. In particular, the combination

$$\gamma \equiv \frac{G_0 T^{1/2}}{n_e}$$

controls the ratio of H_2 to H^0.

As one moves into a PDR, the molecular hydrogen becomes **self-shielding** at column densities $N(\mathrm{H}_2)>10^{14}\ \mathrm{cm}^{-2}$. That is, the radiation in the Lyman and Werner series lines has already been absorbed, so that the FUV radiation that filters into the PDR becomes less efficient (it must excite weaker H_2 lines or operate farther from line center). The rate of photodissociation is then suppressed by a self-shielding factor,

$$\beta_{\mathrm{ss}} \approx \left(\frac{10^{14}\ \mathrm{cm}^{-2}}{N(\mathrm{H}_2)}\right)^{0.75}.$$

In practice, at the surface of a PDR (i.e. at the H^0/H^+ boundary) the reaction rates heavily favor atomic over molecular gas. As one moves deeper into the PDR, the self-shielding of the small amount of H_2 reduces β_{ss} to values <<1 and eventually the gas can become mostly molecular.

3. The Physics of PDRs

A. METALS

Carbon is important because its ionization energy (11.2 eV) is less than that of hydrogen (13.6 eV). Therefore, the radiation that filters through the H^0 zone can still ionize carbon. We found earlier that the unscreened radiation from the central star typically results in an ionized:neutral ratio for H in the H II region of ~few × 10^3, and a similar calculation applies to carbon in the PDR. Therefore we expect carbon (or at least the gas-phase portion) to be primarily in the form of C II. This implies an electron abundance $x_e \sim 10^{-4}$ even though the H and He are neutral.

As one goes deeper into the PDR, dust absorbs the FUV photons and some self-shielding of C I takes place. When the FUV is extincted by a factor of ~10^4 (10 magnitudes, or A_V~4) the carbon becomes mainly neutral. In the C^0 zone, metals with lower ionization potentials (S, Si, Fe, Mg, Na) can be the dominant electron donors.

The transition to neutral carbon is also characterized by the formation of the molecule CO. This is a tightly bound molecule (bond energy ???) and its formation can be catalyzed by a variety of nonradiative molecular reactions starting from O, H_2, and C/C^+. Examples include the sequence involving radicals:

$$\mathrm{O} + \mathrm{H}_2 \rightarrow \mathrm{OH} + \mathrm{H}$$
$$\mathrm{C}^+ + \mathrm{OH} \rightarrow \mathrm{CO}^+ + \mathrm{H}$$
$$\mathrm{CO}^+ + \mathrm{H} \rightarrow \mathrm{CO} + \mathrm{H}^+ .$$

The radicals and CO are susceptible to photodissociation.

B. HEATING

The heating sources in PDRs are all associated either directly or indirectly with the young stars and their UV/optical radiation. The major processes are:

- *Photoelectric effect on dust*: Dust grains (including the PAHs) can undergo the **photoelectric effect**, i.e. the removal of electrons from solids. This is really the same phenomenon as photoionization but applied to bulk material. The ejected electron carries kinetic energy that heats the gas.
- *Carbon photoionization*: This is the analogue of photoionization of H or He in H II regions. It is generally of minor importance compared to dust.

- *Collisional de-excitation of* H_2: Hydrogen molecules excited in the Lyman and Werner bands can decay back to excited vibrational levels of the ground electronic state. At the high densities in PDRs, and given the quadrupole nature of the radiative decays, the H_2 molecules may collisionally de-excite, dumping this vibrational energy into the kinetic degrees of freedom of the gas.
- *Cosmic rays*: These are a subdominant source of heating at the surface of the PDR, but will be significant when we investigate molecular clouds because they can penetrate into the deep interior where UV/optical radiation is shielded.

Since a PDR (defined broadly) absorbs much of the incident ultraviolet radiation through dust, one might expect the photoelectric effect to dominate. This is usually the case at low A_V (indeed it appears to be the case for the diffuse phases of the ISM as well). We will therefore focus on the photoelectric heating.[1]

We define the efficiency of photoelectric heating ε to be the fraction of the absorbed photon energy $h\nu$ that goes into ejected electrons. This is given by

$$\varepsilon = Y \frac{h\nu - W - Z_{\mathrm{d}} e^2 / a}{h\nu},$$

where Z_{d} is the charge of the grain, W is the work function, and Y is the electron yield (i.e. probability that an absorbed photon actually ejects an electron). The charge is significant because in PDRs, the photoelectric process tends to leave grains with a net positive charge, until the electrostatic potential prevents further electrons from leaving and/or attracts electrons from the ambient medium to the grain surface. The yield varies, dropping to near zero for large grains because the photons can penetrate into the deep interior of the grain, while the electrons released there stop due to collisions before they can exit the grain.

For the PAHs, the yield is of order unity. However, even a singly charged PAH (PAH^+) tends to have a second ionization energy exceeding 13.6 eV, so PAH^0 molecules dominate the PAH photoelectric heating. The fraction of PAHs that are neutral tends to be a few tenths (determined by the γ parameter, i.e. the ratio of photon to electron collision rates).

The net efficiency of photoelectric heating varies slowly as a function of T and γ, but values of order $\varepsilon \sim 0.01$ are typical. Given the typical UV dust absorption cross section of $\sim 10^{-21}$ cm^2 per H nucleus, and typical energy flux of $\sim 10^{-3} G_0$ erg cm^{-2} s^{-1}, this suggests a heating rate of $\sim 10^{-26} G_0$ erg/s/H atom.

B. COOLING

The species in PDRs available for cooling are H, O, and C^+; and at greater depths CO. The fine structure lines of O and C^+ are the main coolants since H has no

[1] Tielens §3.3

low-lying excitations (except for the extremely weak 21 cm line). Excitation may be via either electron collisions,

$$\mathrm{C}^+(^2P^o_{1/2}) + e^- \rightarrow \mathrm{C}^+(^2P^o_{3/2}) + e^-,$$

or by neutrals:

$$\mathrm{C}^+(^2P^o_{1/2}) + \mathrm{H} \rightarrow \mathrm{C}^+(^2P^o_{3/2}) + \mathrm{H}.$$

The former reaction has the advantage of Coulomb focusing, and hence has a rate coefficient typically ~100 times larger, but in a mostly neutral region such as a PDR, the latter can be significant. Neither process actually uses the electron spin; rather the 2p electron's orbital angular momentum is changed, or it is swapped for the free electron or that of the H atom.

The excited atoms emit in the [C II] 158 μm and [O I] 63, 146 μm lines. The former has a lower excitation energy (90 K for [C II] 158 μm versus 230 K for [O I] 63 μm), and hence dominates at low temperatures. The latter has a higher critical density (~10^6 cm^{-3} for H collisions) so in dense regions at moderate temperatures it may dominate.

The cooling rate via the 63 μm line is, in the low density limit,

$$2.5\times10^{-29}\, n_{\mathrm{H}}\, T^{0.67}\, \mathrm{e}^{-230\,\mathrm{K}/T}\ \mathrm{erg/s/H\ atom}.$$

We may set this equal to the heating rate to obtain the equation for the temperature:

$$0.0025 n_{\mathrm{H}} T^{0.67} e^{-230\mathrm{K}/T} = G_0.$$

This is a very rough approximation, but it illustrates the main point. At constant pressure, $n_{\mathrm{H}}T = P/k$ = constant, and the left hand side is a slowly falling power law ($T^{-0.33}$) times a rapidly rising exponential. An equilibrium is usually found at temperatures of a few hundred K. There is, however, a maximum of the left-hand side that is proportional to pressure. If the pressure is too low there may not be an equilibrium solution. This is generally not the case in a PDR, but in the diffuse ISM such situations arise and result in runaway heating (until collisional excitation of optical lines takes over). This will be discussed in the lecture on the warm neutral medium.

A final aspect of the problem is that the [O I] line may develop optical depths of order unity in a PDR (column $N_{\mathrm{H}} > 10^{21}$ cm^{-2}). We will not discuss the radiative transfer aspects of the problem here.

4. Diagnostics

We may finally discuss the key diagnostics for PDRs. These have many similarities to the diagnostics for H II regions, but we work at a lower energy and

dust plays a critical role. As always, we must watch out for inhomogeneities – real PDRs are not idealized spherical shells.

A. INCIDENT FLUX

The incident UV flux (or G_0) may be determined by the calorimetry method: the radiation is reprocessed into the FIR, and one may simply take the FIR surface brightness as an estimate of the UV flux. This method requires assumptions about the 3D geometry, which may not be independently known.

An alternative method is to use observations of the central star(s) and use our knowledge of stellar spectra and luminosities as a function of spectral type.

A final method is to use the H_2 fluorescence lines, which are pumped by the FUV continuum. Essentially all incident FUV photons within the spectral lines will be reprocessed by H_2 – unless the incident flux becomes high enough to push the H_2 density to low values, in which case dust can "steal" the FUV photons.

B. DENSITY

The usual method of measuring density is to compare cooling lines of different critical densities. One would like to use two lines of the same species, but the [O I] 63,146 μm fine structure lines have similar critical densities and the former is affected by optical depth effects. [C II] has only a single line.

An alternative, since the O critical density is far greater than the C^+ critical density, is to use the [O I] 146 μm / [C II] 158 μm ratio. This does depend on the O/C^+ ratio, but both of these are majority ionization states and so should trace the general O/C abundance ratio of the ISM (~2:1). At very low temperatures the O lines are suppressed, but this is mainly an issue in cold regions rather than PDRs (≥ 10^2 K).

Molecular rotation lines such as CO could also be used. As J increases, the critical density increases because the radiative rates are faster.

Another way to estimate the density is to measure the heating efficiency ε by dividing the heating rate of the gas (assumed equal to the gas-phase fine structure cooling lines) by the incident flux (from the FIR luminosity). Denser environments will have higher efficiencies because the high electron density implies that the PAH^0/PAH^+ ratio will be higher and the macroscopic grains will have less positive charge.

Yet another method is to note that the structure of a PDR depends on column density, so if its *spatial* structure can be observed one can infer a 3D density.

C. TEMPERATURE

Temperatures in H II regions are typically measured from high-excitation lines such as [O III] 4363Å. In PDRs such techniques would simply probe the ionized-to-neutral transition rather than the bulk of the PDR. One option is to use the [O I] 63 μm line, which if it becomes optically thick can be treated as having

spectral intensity equal to a blackbody. Whether this line is in equilibrium with the gas temperature is a different issue.

Another option is to measure the quadrupole rotation lines of H_2, and infer the population of each J. One can then fit a Boltzmann distribution and infer T. The rotation lines are likely to be in equilibrium with the gas temperature (although the vibrational lines, excited by Lyman/Werner band pumping, may not).

D. MASS

The total mass of gas in a PDR can be estimated from the [C II] 158 μm line. This is typically optically thin ($\tau \sim$ few tenths) and is easily excited (low ΔE, low n_{cr}) so that all C^+ is measured. This is the majority ionization state of carbon so standard abundances can be used to estimate the mass.