PDR'S

This is from the Hollenbach/Tielens (1999, RMP 71, 173; HT) review. To obtain this **and you should get it and read it!)**, go to the RMP web page (*rmp.aps.org/quicksearch.html*) and enter the appropriate vol/page numbers. If you don't follow this procedure you may end up having it tell you that you have to order it for $35.

Other references include Tielens and Hollenbach (1985 ApJ 291 722; TH) high-density PDR treatment ($n = 10^3 \rightarrow 10^6$ cm^{-3}, $G_0 = 10^3 \rightarrow 10^6$); Hollenbach, Takahashi, Tielens (1991 ApJ 377, 192; HTT) low-density, low-radiation PDR's ($n = 10^2 \rightarrow 10^5$ cm^{-3}, $G_0 = 1 \rightarrow 10^4$); Draine & Bertoldi (1996, ApJ 468, 269; DB) improved PDR models; Hollenbach and McKee et al papers for atomic constants (e.g. HM 19889 ApJ 342, 306); also Genzel article for atomic constants.

1. Basic theoretical model of PDR's

PDR's in the ISM have different zones where different species predominate. These include atoms, their ions, and molecules. Radiation (radiative transfer), temperature (heating and cooling processes), and chemistry determine the properties of these zones. But these processes are all interdependent: chemistry depends on temperature and density, temperature depends on the radiation field and species that heat/cool, and the radiative transfer in line radiation (which affects both chemistry and the heating/cooling) depends on the abundances. All this interdependence on complicated microphysical processes makes PDR's impossible to calculate without numerical modeling. We will concentrate on basic microphysical processes that go into these calculations and, also, allow one to make some estimates of physical conditions and where transitions occur.

Classical dense PDR's are summarized succinctly in HT Fig 3, which illustrates a dense PDR (meaning that $\frac{T_0}{n} \gtrsim 0.01$). A neutral slab of gas sits just outside the boundary of an HII region. UV photons (here UV means just under 13.6 ev—they can't ionize HI) dissociate any H_2, CO, and other molecules; ionize C (C IP is 11.3 ev); leave O neutral (O IP is 13.614, H IP is 13.595 ev); $T \sim 100 \rightarrow 1000$ K. The UV attenuates with distance from the boundary, allowing $H \rightarrow H_2$; further in, $C^+ \rightarrow C^0 \rightarrow$ CO, O$\rightarrow O_2$, and further in than that we have a classic molecular cloud. Most of the MW's molecular gas is in the PDR region, not the full molecular region.

The structure of PDR's is governed by the parameter $\frac{G_0}{n(Htot)}$, where G_0 measures the intensity of the radiation field and $n(Htot)$ is the total H-nuclei volume density. $\frac{G_0}{n(Htot)}$ is the governing parameter because the molecules are destroyed by photodissociation, whose rate cm^{-3} scales as G_n, and are formed by binary collisional processes, whose rate cm^{-3} scales as n^2; the ratio is $\frac{G_0}{n}$.

PDR's exist at the boundary of every HII region. Moreover, the diffuse ISM is just a great big PDR (it contains H and C^+). So all of the neutral atomic gas and most of the molecular gas is PDR.

Issues with PDR's:

(1) Gas heating, cooling, equilibrium temp.

(2) H_2 formation and destruction mechanisms. (different regimes).

(3) Scale over which the transitions at the abovementioned interfaces occur. Depends on G_0/n, the radiation field intensity divided by the H-nuclei volume density.

(4) Clumping. Both direct observational evidence and also inferences from departure of theoretical predictions from observations.

2. TWO IMPORTANT FACTORS ABOUT THE RADIATION FIELD

2.1. The Interstellar Radiation Field (ISRF)

The primary heating and H_2-dissociating mechanisms involve electromagnetic radiation. Its mean intensity is usually characterized

$$J_\nu = G_0 \; ISRF_{Habing} \tag{1}$$

where $ISRF_{Habing}$ is the original value for the important range $6 \rightarrow 13.6$ eV, first estimated by Habing (1968) to be 1.6×10^{-3} erg cm^{-2} sec^{-1} $\sim 1.6 \times 10^8$ photons cm^{-2} sec^{-1}. Locally, $G_{0,LOCAL} \sim 1.7$ (Draine 1978) and in PDR's next to HII regions G_0 can reach $> 10^6$.

$ISRF_{LOCAL}$ has an energy density $U = \frac{4\pi J}{c} \sim 7 \times 10^{-13}$ erg cm^{-3}, which is equivalent to blackbody radiation at 3.5 K ($\frac{4\sigma}{c} T^4 = U$) (Spitzer page 194). This is one instance of the strange fact that all interstellar energy densities (cosmic background, gas turbulence, magnetic field, cosmic rays) are characterized by blackbody temperatures near 3 K. But, of course, it's not microwave radiation. It's dilute blackbody radiation, meaning

$$J_\nu = W B_\nu(T^*) \tag{2}$$

where T^* provides the spectral shape and W is the dilution factor. The ISRF is well-approximated by $T_* = 10^4$ K and $W = 10^{-14}$ (Spitzer; Drain 1978); the 10^4 K reflects the fact that, on a dark night, the tradeoff between stars being dimmer with distance and rarer with increasing luminosity means that most of the stars you see are A stars. A better approximation is a superposition of three blackbodies: $(W, T_*) = * * *$ m(I can't find these numbers). Of course, in a PDR this is a poor description because the nearest stars are early-type stars; nevertheless, G_0 remains a useful parameter.

2.2. Extinction by Grains

Grains attenuate the ISRF because of extinction. We will study extinction in detail later, but for now we need to know the properties. Astronomers measure extinction in magnitudes and use the symbol A; one magnitude is a reduction by the factor $100^{1/5} = 2.51 = \frac{e}{1.082}$. Mathematically, one always uses optical depth τ; the reduction factor is $e^{-\tau}$. So $\tau = 1.082$ mag.

For a given dust column extinction decreases with increasing wavelength (same sense as, but much less rapidly than, Rayleigh scattering). This means that dust *reddens* the light, like (but not identical to) the setting sun is reddened by the Earth's atmosphere. This reddening is called selective extinction, denoted by E. All of these quantities need subscripts to define the wavelength. Most commonly, you see $E(B-V)$ meaning the magnitude difference between the extinction at the B and V wavelengths: B is "Blue", centered near 4450 Å, and V is "Visual", centered near 5510 Å(Binney/Merrifield).

We normally assume that the "dust to gas ratio" is everywhere the same. This is not a perfect approximation but it will do for now. This means that $\tau_{gr} \propto N(Htot)$. Moreover, we normally assume "standard dust", which characterizes diffuse interstellar dust. Not all dust is like this. Standard dust has the following characteristics (Spitzer chapter 7):

$$E_{B-V} = \frac{N(Htot)}{5.9 \times 10^{21}} \tag{3a}$$

$$\frac{A_V}{E_{B-V}} = 3.0 \; ; \frac{A_B}{A_V} = \frac{4}{3} \tag{3b}$$

$$\frac{A_{1000A}}{A_V} = 4.33 \tag{3c}$$

$$\tau_{gr,1000A} = 2.4 N(Htot)_{21} \tag{3d}$$

$$\tau_{gr,V} = \frac{N(Htot)}{1.8 \times 10^{21}} \tag{3e}$$

$$\tau_{gr,1000A} = \frac{N(Htot)}{4.2 \times 10^{20}} \tag{3f}$$

In addition to these macroscopic relations involving radiative transfer, there is one more important relationship. The standard gas/dust ratio means that, per H-nucleus, there is a standard grain surface area—important for collision rates with the grains. This is

$$n_{gr}\sigma_{gr} \sim 10^{-21} n(Htot) \text{ cm}^{-2} \; , \tag{3g}$$

where $n(Htot)$ is the number density of H-nuclei, whether neutral, molecular, or ionized.

Comparing the ISM to the Earth's atmosphere, we find that industrial fat cats can make lots more dollars, and add lots more girth to their waistlines, before making Earth's atmosphere as dirty as the ISM. The ISM takes 1.8×10^{21} atoms cm^{-3} to produce optical depth unity in V band. At sea level, the atmosphere has 2.7×10^{19} molecules cm^{-3}, or $\rho = 3.6 \times 10^{-3}$ gm cm^{-3}; you accumulate 1.8×10^{21} atoms cm^{-3} in only 67 cm! If you want to do it in terms of mass density, the atmostpheric mass density at sea level is 1.3×10^{-3} gm cm^{-3}; with the ISM's dust concentration, you reach optical depth unity in only 2.8 cm!!

3. HEATING AND COOLING MECHANISMS; EQUILIBRIUM TEMPERATURE

3.1. Heating

Possibilities that turn out to be unimportant include: cosmic rays (important for ionization in molecular cloud cores, but unimportant in PDR's relative to photons), C excitation/ionization (the classical neutral-gas heating mechanism, which can be important if grains are absent). Heating by hydromagnetic waves might be important in diffuse clouds, but not for dense PDR's). Gas-grain collisions are important where the photon density is too small to dominate the heating—such regions can still be classified as PDR because there are sufficient photons to *dissociate* and *ionize.*

In this discussion we omit heating by gasdynamical processes, including thunder and hydromagnetic waves; their importance is probably limited to the diffuse ISM, and we will cover them later. We also ignore ambipolar diffusion, whose importance is limited to dense molecular regions. Among the microphysical processes, the important and/or interesting processes include:

3.1.1. Photoelectric Heating by C-atom Ionization

This process isn't very important unless the grains are ineffective. We include it because, under some circumstances in the diffuse (low-density) neutral interstellar medium, grains are absent and then this process dominates.

The IP of CI is 11.26 ev, well below the 13.6 ev of HI. There are plenty of photons to ionize CI and, in fact, most of the CI is CII unless the starlight is highly attenuated. The heating rate is

$$n\Gamma_C = \text{ionization rate} \times \text{energy released per ionization} \tag{4}$$

In statistical equilibrium, the ionization rate equals the recombination rate. The recombination rate is $n_e n(CII)\alpha$. But there is enough starlight to make C (almost) fully ionized, so that $n(CII) = n(Ctot)$. Moreover, when H is neutral the electrons come only from ionized heavy elements—and C is by far the most abundant heavy element with $IP < 13.6$ ev. Thus we take $n_e n(CII) =$

$n(C)^2 = \mathcal{A}(C)^2 \delta_{gr}^2 n(H)^2$, where $\mathcal{A}(C)$ is the cosmic abundance of C relative to H. We introduce the *depletion factor* $\delta_{C,gr}$: this accounts for the fact that some of the Carbon is soaked up in the grains and is thus not available in the gas phase. $\delta_{C,gr} < 1$, perhaps 0.5; we discuss it detail later.

Assume the hydrogenic approximation (excluding the $n = 1$ state: it's already occupied) for the recombination; from Spitzer's page 107, we estimate $\alpha = 7.0 \times 10^{-12} T_2^{-0.7} =$ cm^3 s^{-1}. Moreover, the ISRF has a color temperature $T^* \sim 10^4$ K; we found in our earlier studies of HII regions that the energy released per photoionization at this temperature is $\sim 1.2kT^*$ (but this needs to be increased in HI regions to allow for photons between 11.26 and 13.6 ev; 2 ev is a reasonable number). Putting all this together with $\mathcal{A}(C) = 4 \times 10^{-4}$,

$$n\Gamma_C \approx 4.1 \times 10^{-30} \delta_{C,gr}^2 n(Htot)^2 T_2^{-0.7} \text{ erg cm}^{-3} \text{ s}^{-1} \ . \tag{5}$$

As we shall see, this is much smaller than the heating from grains under normal circumstances.

3.1.2. Photoelectric Heating by Grain Ionization

Photoelectric ionization of a grain is like that of an atom, or a photomultiplier cathode. An incident photon ejects an electron, whose energy exceeds the average energy ($\frac{3}{2}kT$) of the gas particles, so it's a heater. Energy of ejected electron equals photon energy minus grain ionization potential minus the charged grain's electrostatic potential. The most effective grains for heating are the very small ones with size $\lesssim 50$ Å.

$$n\Gamma_{dust} = (n_{gr}\sigma_{gr}) \int_{E_{th}/h}^{13.6ev/h} \left(\frac{4\pi J_\nu}{h\nu} \right) Q_a y E_2 d\nu \tag{6}$$

where (n, σ) are the volume density and cross section; $\left(\frac{4\pi J_\nu}{h\nu}\right)$ is the photon flux; $Q_a \sim 1$ the absorption efficiency of a grain for the photons; y the photoelectric yield, ~ 0.1 for large grains and much higher for smaller grains; and E_2 the energy of the ejected photoelectron.

$$E_2 = h\nu - (work\ fcn) - (columb\ barrier) \tag{7}$$

Typically $(work\ fcn) \sim 6 \rightarrow 8$ ev. $(colomb\ barrier) = \frac{n_{el} e^2}{r_{grain}} \sim 1$ ev for one electron-charged grain and a 20 Ågrain (classical electrostatic potential).

Lets put in some numbers. First, take the standard dust/gas ratio, meaning that the dust grain surface area per unit volume is directly proportional to the H-nuclei volume density: $n_{gr}\sigma_{gr} \sim 10^{-21} n(Htot)$ cm^{-2}. Then take the mean photon intensity $\int_{E_{th}/h}^{13.6ev/h} \left(\frac{4\pi J_\nu}{h\nu}\right) d\nu = 1.6 \times 10^8 G_0$ cm^{-2} sec^{-1}. Take the product of the efficiency factors equal to 0.5 and take $E_2 = 1$ ev $= 1.6 \times 10^{-12}$ erg. This gives

$$n\Gamma_{dust} \approx 1.3 \times 10^{-25} n_{Htot} \text{ erg cm}^{-3} \text{ s}^{-1} \tag{8}$$

We've omitted some very important details. The efficiency factor depends on conditions. In strong radiation fields or small electron density, the grain photoejection rate is limited not by the starlight intensity but instead by the recombination rate of electrons onto grains. In this case, the heating $\propto \alpha_{gr} n_e n_{gr}$, where α_{gr} is the recombination coefficient of the grains; as is usual for charged particles, $\alpha_{gr} \propto T_e^{-1/2}$.

And if the gas is warm enough and the radiation field cool enough, then the recombination of thermal grains onto the grains can cool the gas because they give up more energy than they inject into the gas during the photoejection process. This cooling is particularly important for the Warm Neutral Medium: it limits the temperature to $\lesssim 10^4$ K (Bakes and Tielens 1994).

HT give a net efficiency factor for the grain heating efficiency, which is obtained from Bakes and Tielens (1994 ApJ 427, 822). Their equation (41) and Figure 11 give the *photoelectric heating efficiency* ϵ; see attached page.

$$\epsilon = \frac{3 \times 10^{-2}}{1 + 2 \times 10^{-4} \frac{G_0 T^{1/2}}{n_e}} \tag{9}$$

where T is in K and n_e in cm^{-3}. HT give a more complicated formula, which is presumably better. For an HII-region PDR with $n(H) = 10^4$ cm^{-3}, $T = 100$ K, $G_0 = 10^4$, and $x_e = \frac{n_e}{n(H)} = 10^{-4}$ we have $\frac{G_0 T^{1/2}}{n_e} = 10^5$, so the second term dominates the denominator. This illustrates that the grains are starved for electrons—the heating is recombination limited.

This efficiency is equal to the heating rate divided by the total radiation hitting the grain. The remainder of the radiation hitting the grain simply heats the grain. This energy is subsequently re-radiated in the IR. Thus, one can measure the efficiency by comparing the cooling radiation from IR FS lines (equal to the heating rate) to the continuum IR emission from the grains (grain heating rate). Values in the region M17 $\sim 0.25\%$ (Meixner et al 1992 ApJ 390 499). In contrast, in M16 Levenson et al (2000 ApJ 533 L53—Berkeley group!) find 4%. So the conditions really do matter.

In the Galactic-average diffuse ISM, the COBE measurements of the CII line and the dust IR provide an efficiency of 0.3%. The total dust emission implies $G_0 \sim 50$, and for a typical diffuse cloud density $n(HI) = 30$ cm^{-3} and $T = 100$ K they predict 0.3% too!

Bakes and Tielens discuss the solid state physics and processes relevant to ionization of PAH grains containing ~ 100 C atoms. The photoionization occurs of the C atoms in the grain. The heating efficiency drops rapidly for grains having more than ~ 1000 C atoms (Figure 8). This is a result of the fact that the UV absorption cross section $\propto N_C^{2/3}$, where N_C is the number of C atoms in the grain (I guess this is grain surface area), but the recombination scales as $N_C^{1/3}$

(linear with grain size—why?), meaning that large grains have more charge and are less efficient. About half the heating is from grains with $N_c \lesssim 1500$ (grain radius 15 Å); the other half is from $N_c = 1500 \rightarrow 4.5 \times 10^5$ ($a = 15 \rightarrow 100$ Å).

Seems to me this sensitivity to small grains is very important in dense regions like PDR's, where I'd expect the small grains (PAH's) to coagulate onto larger ones. Nevertheless, this doesn't happen. The PAH's emit the Unidentified InfraRed (UIR) bands, features at 3.3, 6.2, 7.7, 8.6, and 11.3 μm (HT Figure 11). These bands also exist from diffuse ISM (the famous 12 μm emission discovered by IRAS), showing that the emission comes from grains that can be regarded as large molecules (otherwise, the starlight energy striking it would be dissipated in phonon modes in the solid state).

The ratio of energy emitted in the UIR bands to the total continuum IR is about 5%. The total continuum is emitted by larger grains that are true solids. So about 5% of the net energy absorbed by grains goes into PAH's. This allows one to calculate how much of the total interstellar C is in PAH's: it's $\sim 1\%$, very small.

3.1.3. H_2 ejection from Grains

H_2 is formed on grains. It takes a few ev to escape and the H_2 binding energy $\gtrsim 10$ ev, so most of the chemical energy released goes, with the ejected H_2, into the gas. Below we treat this process in more detail; here we simply state that

$$n\Gamma_{H2} \sim 5 \times 10^{-28} n(Htot) n(HI) \text{ erg cm}^{-3} \text{ s}^{-1} \ . \tag{10}$$

You'd think that at high densities this would dominate grain heating; however, at high densities most of the H is molecular. I don't know the relative importance here.

3.1.4. H_2 Excitation as a Heat Source

UV photons excite H_2 to excited electronic states. It then decays, with some dissociating (probability ~ 0.1) and the rest coming down into an exited vibrational state having energy ~ 2 ev. Mostly, these decay to the ground states by radiating roto/vibrational lines in the near IR. But at high densities some of these are collisionally de-excited, and heat the gas. See HT.

3.2. COOLING MECHANISMS

We observe these cooling transitions directly both in the radio and IR.

3.2.1. Near the boundary, IR FS lines

Near the boundary of the PDR, where there are no molecules, IR FS structures lines of CII and OI are the primary coolants under almost all circumstances (158 and 63 μm, respectively; HT Fig 16). Exception: For high G_0 and n, which can occur just at the HII region boundary, the temperature can reach thousands of K, high enough to collisionally excite OI 6300 Åand SII 6730 Å; this is one of those rare instances where these lines should be observable (Störzer & Hollenbach 2000, ApJ 539, 751). These FS IR lines are observed directly, but from above the atmosphere or, using an airplane (KAO [Kuiper Airborne Observatory)] or, soon, SOFIA), from above most of it.

For any line under the conditions of low density and small optical depth, we have

$$n^2\Lambda = n_{coll} n_{atom} \gamma h\nu \tag{11}$$

where n_{atom} is the number density of atoms or ions for the transition and n_{coll} is the density of colliding particles. For example, using RG's parameters for the CII 158 μm line and the collider being HI, we have

$$n^2\Lambda = 8.7 \times 10^{-27} n(Htot)^2 \delta_{C,gr} e^{-92/T} \text{ erg cm}^{-3} \text{ s}^{-1} \ . \tag{12}$$

H_2 has a smaller cross section and half the number of colliding particles, so you have to use a different constant.

As you go into the PDR, CII→CI and then, further in, CI→CO. In the CI region, CI is the primary coolant; its FS lines are 609, 370 μm with $n_{crit} \sim (470, 1200)$ respectively. The first line has 490 GHz and is accessible by terrestrial radio astronomy. But at these high frequencies, you need an excellent site; as far as I know, only the Mauna Kea Caltech Submillimeter Observatory (CSO) and South Pole (ASTRO telescope) can observe them. The second line at 810 GHz is also, barely, observable at least from South Pole (don't know about Mauna Kea).

3.2.2. Two important physical details for cooling radiation

Above we emphasized that the cooling rate given applies in the optically thin, low-density case. These are two important issues with cooling lines. This is often particularly important for the FS IR lines, which have lower critical densities and are often emitted in regions where densities are smaller than critical. For example, critical densities for CI and OI lines are 3×10^3 and $\sim 8 \times 10^5$ cm^{-3}, respectively.

Optical depths can be high and reduce the cooling rates. This falls under the general area of radiative transfer. Radiative transfer is simple when $\tau \ll 1$ or when collisions dominate the excitation. Otherwise, one needs to worry about photon trapping; see our writeup on radiative transfer. Approximations for radiative transfer always assume something about the velocity field, because that determines how easily photons can leave, and the assumptions might not apply in a particular case, making big differences (see HT comments at top of page 191).

For an exact solution of the resonance line problem when there are no velocity gradients: Neufield (1990 apj, 350,216).

3.2.3. Further in, molecular lines

Going further in, to the CO region, gives us as the primary coolant with its rotational lines. The low-J transitions are easily observable by terrestrial radio astronomers. But in the warmer, denser regions the higher J transitions lie in the IR. For example, in CO the $J = 7 \rightarrow 6$ transition traces $(n(Htot), T) = (10^5\ \mathrm{cm}^{-3}, 150\ \mathrm{K})$; the $J = 14 \rightarrow 13$ traces $(n(Htot), T) = (10^7\ \mathrm{cm}^{-3}, 500\ \mathrm{K})$; and even the $J = 17 \rightarrow 16$ transition has been observed.

At more extreme densities, vibrational and rotationally excited H_2 is significant. All these are in the near/far IR; we won't discuss these conditions in this course.

Some notes on spectra of diatomic molecules:

3.2.4. Gas-Grain Collisions (Can Also Be a Heating Mechanism!)

We follow Burke and Hollenbach (1983 ApJ 265, 223; BH). If gas particles collide with a grain and come off with the grain's temperature, then the cooling rate is

$$n^2\Lambda = (n_{gr}\sigma_{gr})n_{gas}V_{th}\bar{\alpha_T}(2kT_{gas} - 2ktT_{gr}) \tag{13}$$

where V_{th} is the gas thermal velocity and n_{gas} is the volume density of gas particles. From kinetic theory, $2kT$ is the appropriate average of energy for the incident gas particles. $\bar{\alpha_T}$ is an efficiency factor. A bit of care is required for the gas particles: H-atoms stick below $T_{gr} \sim 100$ K so are not effective, leaving He and H_2. For those, one must insert appropriate thermal velocities

$$V_{th} = \left(\frac{8kT}{\pi m}\right)^{1/2} \tag{14}$$

where m is the appropriate mass. BH show that $\bar{\alpha_T} \sim 0.6$. Putting in all the numbers, we get

$$n^2\Gamma \approx 1.2 \times 10^{-32} T_2^{1/2} n(Htot)^2 (T_{gas} - T_{gr}) \text{ erg cm}^{-3} \text{ s}^{-1} \ . \tag{15}$$

This is important only at large densities and, even then, only when the gas and grains are at significantly different temperatures—facts that are not appreciated by some astronomers.

3.3. Results: Equilibrium gas temp

At the entrance to PDR, temp can be $500 \rightarrow 1000$ K because of relatively intense UV photon field and its heating, or even higher with extreme G_0. Moving away from the edge (measured in τ_{dust} units, usually expressed in terms of A_V), T drops gradually and at $A_V \sim 4$, the UV photons are gone so there's no dust or H_2heating: heating is from gas-grain collisions (*not* photoelectric grain heating), cooling still from CII and OI, equilibrium T drops to ~ 30 K, and grains are a bit warmer than the gas (as they must be to act as a collisional heat source).

4. H_2 FORMATION AND DESTRUCTION

4.1. H_2 Formation

The basic process: An H atom hits the grain, sticks, wanders around until it is trapped in a potential well. This happens until all the wells are full. During and after this, an arbitrary incoming H will, during its wanderings, encounter another H. When this happens, they form H_2, which requires a third object to conserve energy and angular momentum; this object is the grain.

The H_2 is then ejected. The chemical formation of H_2 releases energy; a few ev goes to the grain and most goes into internal excitation of the H_2 and kinetic energy.

The H_2 formation rate is thus $\propto n(HI)n_{gr}$. More specifically, realizing that it takes two HI's to make an H_2,

$$R_{form} = \frac{(n_{gr}\sigma_{gr})\ (n_H v_H)}{2} S(T, T_{gr})\eta(T_{gr}) \tag{16}$$

where $S \sim 1$ is H-sticking probability, $\eta \sim 1$ is probability that a stuck-H atom finds another H to form H_2; both of these are nearly unity. Putting in numbers, we adopt HT's numbers,

$$R_{form} = 3 \times 10^{-17} n(Htot)n(HI)T_2^{1/2} \mathrm{cm}^{-3}\ \mathrm{s}^{-1}\ . \tag{17}$$

Thus the time scale to convert e^{-1} of the HI to H_2 is

$$\tau_{HI \rightarrow H2} = \frac{6\ Myr}{n(Htot)_2 T_2^{1/2}} \tag{18}$$

where $n(Htot)_2$ means total H nuclei volume density in units of 100 cm^{-2}. In dense PDR's ($n(Htot) \sim 10^5$ cm^{-3} is not uncommon) this is virtually instantaneous, but in the diffuse PDR of typical interstellar space it's nontrivial and too long for some clouds.

For gas heating, assuming a kinetic energy of 10 ev we recover equation 10.

4.2. H_2 Destruction

Destruction of H_2 is by a special type of photodissociation. Ordinarily, we think of photodissociation as akin to ionization, so UV continuum destroys the molecule. But H_2 dissociates through the absorption of spectral line photons, as shown on accompanying notes. These lines get optically thick with relatively small H_2 column densities. Hence, the H_2 shields itself: "self-shielding". It's like the boundary of an HII region, where HI shields itself (but HI ionization occurs with continuum, not line, of course). See the attached handwritten figure and notes for more.

Write the photodissociation rate in the absence of any attenuation by extinction or self-shielding as $R_{diss} = I_{diss} n_{H_2}$ cm^{-3} sec^{-1}; the dissociation rate $I_{diss} \sim 4 \times 10^{-11}$ sec^{-1}(see hand-written notes). Then the grain attenuation of radiation is τ_{gr} (1000 Å is the relevant wavelength). Let the attenuation by self-shielding be f_{ss}; then we have (HT eqn 5)

$$R_{diss} = [f_{ss}(N(H_2))]\ e^{-\tau_{gr}} I_{diss} n_{H_2} \tag{19}$$

where we write $[f_{ss}(N(H_2))]$ to emphasize that the self shielding depends only on H_2 column density from edge.

Consider the ratio of the formation rate (at the edge of the cloud where the incident UV hits) to the four times unattenuated dissociation rate:

$$\mathcal{R} = \frac{R_{form}}{4I_{diss}} = 1.9 \times 10^{-7} T_2^{1/2} \frac{n(Htot)}{G_0} \tag{20}$$

(The factor 4 makes the following expressions simpler). *This quantity, $\mathcal{R}$, is very important.* Its tiny value shows that H_2 will only be abundant if $G_0/n \ll 1$. In other words, to get significant H_2 abundance, we need to attenuate the UV is attenuated by a huge factor, $\sim 10^7/n$.

4.2.1. H_2 self shielding

One derives f_{ss} from the amount of radiation getting through highly saturated absorption lines. This depends on macroscopic velocity structure; no multiple velocity components give

$$f_{ss} \sim \left(\frac{N(H_2)}{10^{11}\ \mathrm{cm}^{-2}} \right)^{-1/2} \tag{21a}$$

The inverse square-root behavior occurs because the absorption lines are saturated, so their equivalent widths are on the classic "square-root" portion of the curve. For details of this, see handwritten notes. However, DB show that overlapping of these lines increases f_{ss}, resulting in a more complicated behavior (their Figs 3 $\rightarrow$ 7) that can be roughly approximated by

$$f_{ss} \sim \left(\frac{N(H_2)}{10^{14}\ \mathrm{cm}^{-2}} \right)^{-3/4} = \left(\frac{N(H_2)}{N_0} \right)^{-3/4} \tag{21b}$$

These look much different but give comparable answers for $N(H_2) = 10^{20} \rightarrow 10^{21}\ \mathrm{cm}^{-2}$, which is where it matters.

Note how effective self-shielding is!!! A column of only $N(H_2) = 10^{20}$ reduces the photodissociation rate by $\sim 3 \times 10^4$! In contrast, the reduction by dust is only a factor of 1.6. Nevertheless, dust can be important.

Notes on why the self shielding goes as $N^{-1/2}$ for the case of nonoverlapping lines:

4.2.2. Self-shielding dominant case

For small enough $\frac{G_0}{n(Htot)}$, self shielding dominates. Take (formation, destruction) as

$$\frac{dn(H_2)}{dt} = \gamma n(HI)n(Htot) \tag{22a}$$

$$\frac{dn(H_2)}{dt} = -n(H_2)I_{diss}\left(\frac{N(H_2)}{N_0}\right)^{-3/4} \tag{22b}$$

So we are neglecting the dust opacity. Set these equal:

$$N(H_2)^{-3/4}n(H_2) = \frac{\gamma n(Htot)}{4I_{diss}}n(HI)N_0^{-3/4} \tag{23}$$

and realize that along path length s from the edge of the region, we have

$$n(H_2) = \frac{dN(H_2)}{ds} \tag{24}$$

$$N(H_2) = \int n(H_2)ds \tag{25}$$

so

$$N(H_2)^{-3/4}n(H_2) = \frac{4dN(H_2)^{1/4}}{ds} \tag{26}$$

There are two interesting ways to write the results:

(1) For an ordinary diffuse interstellar cloud one has $G_0 \sim 1$ and $n(Htot) \sim 100$ cm^{-2}, so $\frac{G_0}{n} \sim 0.01$. We measure $N(HI)$ directly from the 21-cm line for such clouds, and most astronomers who do so assume they see all the mass—that all H is HI. Is this correct? We write the above in the form

$$\frac{N(H_2)}{N_{HI}} = \left(\frac{\gamma n(Htot)}{4G_0 I_{diss}}\right)^4 \left(\frac{N(HI)}{N_0}\right)^3 \tag{27}$$

Plug in values $\gamma = 2 \times 10^{-17}$ cm^3 sec^{-1}, $I_{diss} = 4 \times 10^{-11} G_0$, $N_0 = 10^{14}$ cm^{-2}, to get

$$\boldsymbol{\frac{N(H_2)}{N(HI)} = \left(\frac{n(Htot)_2}{G_0}\right)^4 \left(\frac{N(HI)_{20}}{3.5}\right)^4} \tag{28}$$

This is interesting for ordinary interstellar HI clouds. If one measures, with the 21 cm line, $N(HI)_{20} = 3.5$ (generally considered a modest HI column density) and if $n(Htot) = 100$ cm^{-3}, then $N(H_2) = N(HI)$. Remembering that H_2 contains two H atoms, this means that $\frac{2}{3}$ of the cloud's H—most of its mass—is molecular. Thus, if there is time for equilibrium to establish, interstellar clouds studied in the 21-cm line might be mainly H_2!

Reach, Koo, and Heiles (1994 ApJ 429, 672; RKH) determined H_2 column densities by subtracting HI column densities from the IRAS 100 μm maps, using the standard ratio between total column density and 100 μm brightness. They found good agreement with the above relationship. In particular, for a particular cloud known as G236+30 they found significant H_2 abundances for $N(HI) \gtrsim 3.4 \times 10^{20}$ cm^{-2} for $n(Htot) = 50$ cm^{-3} assuming $T = 80$ K. More generally, they find that for a typical cloud one expects

$$\frac{M(H_2)}{M(HI)} = \left(\frac{n(Htot)}{50 \text{ cm}^{-3}}\right)\left(\frac{T}{80 \text{ K}}\right)\left(\frac{\langle N(HI)^2\rangle}{\langle 4 \times 10^{20} N(HI)\rangle}\right) , \tag{29}$$

where the angle brackets indicate averaging over the entire cloud. Note that this relationship normalizes so that the thermal pressure is $\frac{P}{k} = 4000$ cm^{-3} K, which is the typical value. They caution that this applies only if the H_2 formation process has had time to come to equilibrium.

RKH also measured CO emission and found that the formation of CO required more like $N(Htot) \sim 10^{21}$ cm^{-2}, in agreement with the PDR model, which predicts different transition points for the two molecules (with CO coming on for higher columns). This proves that the fabled CO/H_2 ratio, often denoted X, the value of which some radio astronomer expend lots of energy arguing about, is intrinsically not a constant.

(2) For thinking and making rough calculations about PDR's, we can write

$$\frac{N(H_2)}{N(Htot)} = \left(\frac{\gamma n(HI)}{4I_{diss}}\right)^4 \left(\frac{N(Htot)}{N_0}\right)^3 \tag{30}$$

And then we can pull a swindle: for regions in front of the HI-H_2 transition zone, most of the H is HI so we can replace $n(HI)$ by $n(Htot)$. This puts things entirely in terms of $n(Htot)$, which is nice because we can use the parameter $\mathcal{R}$:

$$\frac{N(H_2)}{N(Htot)} = \mathcal{R}^4 \left(\frac{N(Htot)}{N_0}\right)^3 \tag{31}$$

In addition, define $x_{H_2} = \frac{n_{H2}}{n(Htot)}$ and, realizing that

$$x_{H2} = \frac{dN(H_2)}{dN(Htot)} \tag{32}$$

we can write

$$x_{H_2} = 4\mathcal{R}^4 \left(\frac{N(Htot)}{N_0}\right)^3 \tag{33}$$

This is an important equation: x_{H_2} goes as $N(Htot)^3$, so the transition zone is very sharp. Intrinsically, that's because f_{ss} becomes huge as soon as a tiny $N(H_2)$ builds up.

The **T**ransition **Z**one, where half the gas is molecular, has $x_{H_2} = \frac{1}{4}$, which occurs at

$$N_{TZ} \sim 0.4A^{-4/3}N_0 = 6.4 \times 10^{22} \left(\frac{G_0}{n(Htot)}\right)^{4/3} \text{ cm}^2 \tag{34}$$

Note: HT give 5.0 instead of 0.4; this is a typo. In terms of UV extinction, this is

$$\tau_{1000} \sim 151 \left(\frac{G_0}{n(Htot)}\right)^{4/3} \tag{35}$$

Recall that we have neglected dust…

4.2.3. Dust-dominant case

At the transition point $x_{H_2} = \frac{1}{4}$, self-shielding always dominates dust absorption. That's because self-shielding is so strong: for $N(Htot) = 10^{20}$ cm^{-2}, $f_{ss} \sim 3 \times 10^{-5}$. But the self shielding, which allows H_2 to survive, requires the presence of H_2. Even a tiny amount will act as a catalyst, reducing f_{ss} to allow the rapid buildup of more H_2. According to equation 34, generating this initial little bit of H_2 requires a large column density $N(Htot)$ unless $\left(\frac{G_0}{n(Htot)}\right)^{4/3}$ is small.

If the required column density $N_{TZ,21} \gtrsim 0.5$, then dust becomes important because $\tau_{1000} \sim 1$ for $N(Htot)_{21} \sim 0.5$ (recall $\tau_{1000} = 2.4N(Htot)_{21}$). When this happens, the dust opacity will allow the tiny little bit of H_2 to form; self shielding then develops rapidly and the transition point soon follows. Setting $N_{TZ,21} \sim 0.5$, dust determines the transition point when

$$\frac{G_0}{n} \sim 0.026 \tag{36}$$

and **the transition point occurs near $\boldsymbol{N(Htot)_{21} \gtrsim 1}$** (a few $\times 10^{21}$; higher values for higher G_0).

4.3. Summary Statement

The structure of the PDR depends on the ratio $\frac{G_0}{n(Htot)}$. For $\frac{G_0}{n} \gtrsim 0.026$, dust opacity decreases H_2 destruction enough to allow H_2 to build up near $N(Htot)_{21} \sim 1$ and the transition to H_2 occurs at a few times this. For smaller $\frac{G_0}{n}$, the transition occurs at lower $N(Htot)$. Diffuse clouds in the ISM have $\frac{G_0}{n} \approx \frac{1}{n(Htot)}$ and are almost always in the latter category.

While the UV flux at the edge of HII regions is often high (Orion has $G_0 \sim 10^5$), the density is also high ($\sim 10^5$ cm^{-3} for Orion bar), so $\frac{G_0}{n(Htot)}$ can take on a wide range of values. For Orion, the transition is dominated by dust, so the HI-H_2 transition occurs occurs near $A_V \sim 4$ mag ($N_{Htot,21} \sim 5$). OI and CII cooling lines are brightest in the HI region and fall drastically a bit further in than the H_2 boundary. (HT Fig 16). In the H_2 zone, cooling is dominated by CO rotational lines and a bit of CI FS emission.

5. DENSITIES, TEMPERATURES, AND CLUMPING

5.1. Evidence for clumping

Consider Orion. In HT Table II, Lines provide two density regimes, $(n, T) \sim (5 \times 10^4$ cm$^{-3}, 500$ K$)$ and $(n, T) \sim (1 \times 10^7$ cm$^{-3}, 2000$ K$)$. OI and CII FS lines come from the low-density part and are extended over angle ~ 5 arcmin. At Orion's 500 pc distance, this is about 0.6 pc $\sim 2 \times 10^{18}$ cm, so with $n(H) = 5 \times 10^4$ cm^{-3} the column density $\sim 10^{23}$ cm^{-2}. This corresponds to $A_V = 55$ mag., which means that the concept of photons getting in to keep H_2 dissociated is absurd. Therefore, the extended nature of the *interclump* gas implies that it has a lot of structure; the surface might be corrugated so as to allow photons to penetrate large distances without being absorbed.

The CII line has low critical density and is thermalized in any PDR associated with an HII region. PDR models show that the CII$\rightarrow$CI transition occurs at $A_V \sim$ a few, or $N(H) \sim 10^{22}$ cm^{-2}. A typical PDR has interclump $n(H) = 3000 \rightarrow 50000$ cm^{-3}; so the CII should disappear in a length $\sim 1 \rightarrow 0.05$ pc. Most of the mass is in the clumps; if the mass were uniformly distributed, this distance would be much shorter.

Radio C91α line indicates $n \sim 10^6$ towards Orion exciting star; spectra show a bright, narrow line. Advantage in radio is accuracy of velocity measurements (Natta, Walmsley, Tielens ApJ 428, 209. GOOD PROJECT: try Zeeman splitting of these C lines!!!!!!!

Moreover, there's lots of evidence for dense clumps mixed in with the interclump gas. High-excitation lines include CO J=14-13, radio recombination lines of C, and H_2 J=1-1 plus others. Also, one sees clumps directly in radio maps of molecular emission and, also, FIR emission from grains.

The clumps are important in themselves. Also, they modify the radiative transfer of the sub-UV photons within the PDR.

5.2. Physical Properties of Clumps and Interclump

In *Orion Bar*, from HT Table II: Interclump $(n, T) \sim (5 \times 10^4, 500)$, with $\frac{P}{k} = 2.5 \times 10^7$ cm^{-3} K. Clump $(n, T) \sim 10^7, 2000$; $\frac{P}{k} = 2 \times 10^{10}$ cm^{-3} K . So the clumps are highly overpressured.

In *M17* (Meixner et al 1992 ApJ 390 499), Interclump $(n, T) \sim (3000, 200)$, with $\frac{P}{k} = 6 \times 10^5$ cm^{-3} K. Clump $(n, T) \sim 5 \times 10^5, 1000$; $\frac{P}{k} = 5 \times 10^8$ cm^{-3} K . So again the clumps are highly overpressured. Properties vary a lot from one region to another.

5.3. Extreme clumping: OH and CH_3OH masers

Three types of masers are commonly found in HII region vicinities.

H_2O masers are the strongest. They are seen over huge velocity ranges (often several hundred km/s) and VLBI studies show they are expanding from a certain point. This point is a massive star. These things are tiny, as small as $\sim 10^{13}$ cm (about 1 AU!) with $n(H2) \sim 10^8 \rightarrow 10^{10}$ cm^{-3}; brightness temperatures range up to 10^{15} K (!). So during the process of massive star formation, these things get ejected. By using VLBI to measure proper motions and combining with Doppler shifts, one does "statistical parallax" to get accurate distances. Problem is that the velocity distribution may be anisotropic...stars tend to eject things along their rotational poles.

H_2O megamasers in extragalactic sources are observed. VLBI observations allow measurements of the proper motions and Doppler velocities; combining these with models of the orbits provides the most accurate extragalactic distances ever measured. Problem: only one object so far! These masers are probably the result of an X-R dissociation region having $n(H) \sim 10^9$ cm^{-3}.

OH and CH_3OH masers are observed in PDR's around HII region. OH masers are larger than H_2O masers, typically $10 \rightarrow 100$ AU, with T_B up to 10^{13} K; CH_3OH masers are larger with smaller brightness temperatures. Maser theory implies OH masers have $n(HI) \sim 10^8$ cm^{-3} and $T_K \sim 100$ K, so $\frac{P}{K} \sim 10^{10}$ cm^{-3} K. Details of maser formation are not perfectly well understood.

5.4. Clump stability: Virial Theorem

Virial theorem: Neglecting surface terms and magnetic field, we have the virial theorem, which is the condition required for stability:

$$PE + 2KE = 0 \tag{37}$$

where PE is gravitational PE and KE is kinetic energy. As a simple application, a planet of mass m orbiting a star of mass M at distance R: $PE = -\frac{GMm}{R}$ and $KE = \frac{mv^2}{2}$. This balances centrifugal and gravitational force: $\frac{v^2}{R} = \frac{GM}{R^2}$ so it actually works.

For a uniform spherical clump of mass density ρ, radius R, and velocity dispersion δv, we have $M = \frac{4\pi}{3}\rho R^3$, $PE = -\frac{3}{5}\frac{GM^2}{R}$. We have $2KE = M\delta v^2$. This gives

$$\rho = \frac{5}{3}\frac{\delta v^2}{GR^3} \tag{38}$$

or, putting in numbers,

$$R \sim 0.05 \frac{\delta v_{km/s}}{n(H)_6^{1/2}} \text{ pc} \tag{39}$$

where $n(HI)_6 = \frac{n(HI)}{10^6}$. The M17 clumps have observed sizes $\sim$ 0.1 pc, which makes them "gravitationally bound" (the euphonism for being in virial equilibrium). Ditto for OH masers. Of course, these clumps it *have* to be virialized if the observed clumps are not going to explode: they are high pressure clouds sitting in a low pressure environment. It would seem, then, that the clumps are incipient stars. Probably pre-existing in the original molecular cloud before the ionization/shock front swept over it. Or, perhaps, an instability in the ionization/shock?

6. CLUMPING AND RADIATIVE TRANSFER

Clumping modified the radiative transfer. Basically, the effective absorption coefficient is reduced by an amount that depends on the clumping details. This can be a huge effect, and allows dense PDR's to be much larger than they would otherwise be. Another effect of the clumping is to create a large dispersion in the UV photon flux at any one depth. See HT §IIA and Figures 6 and 7. Also the attached notes.

Some notes on the effective absorption coefficient in a clumped medium: