

PHOTON-DOMINATED AND X-RAY DOMINATED REGIONS

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Abstract. A brief account is presented of the chemical characteristics of regions controlled by the absorption of X-rays. Recent studies of the infrared emission from molecular hydrogen and time-dependent effects in evolving photon-dominated regions are summarized.

1. Introduction

Photon-dominated regions or photodissociation regions (PDRs) are regions of gas exposed to far ultraviolet radiation. PDRs occur at the boundaries of HII regions and planetary and reflection nebulae, on the edges of and inside clumpy molecular clouds, in starburst galaxies and in the narrow line regions of active galactic nuclei (Stacey et al. 1993, Van der Werf et al. 1993, 1996, Zhou et al. 1993, Störzer, Stutzki & Sternberg 1996, Luhman & Jaffe 1996, Luhman & Rieke 1996). Because of absorption by H₂ and by grains, PDRs are limited in spatial extent and they exist as narrow interfaces, separating ionized and neutral material.

X-ray dominated regions or X-ray dissociation regions (XDRs) are regions of gas exposed to X-rays. XDRs occur in molecular clouds with embedded X-ray sources, in active galactic nuclei and near to supernova remnants and high velocity shocks. X-ray absorption cross sections diminish

rapidly at high photon frequencies and XDRs may extend over large spatial dimensions.

In PDRs, molecular formation is driven by photoionization and molecular destruction by photodissociation. In XDRs, molecular formation is again driven by photoionization but destruction occurs through ion-molecule reactions and by the secondary effects of the energetic photoelectrons, including photodissociation by the absorption of internally generated ultraviolet photons.

Both PDRs and XDRs contain zones of enhanced temperature in which endothermic reactions with H_2 contribute significantly to molecular formation. Both PDRs (Black & Dalgarno 1976) and XDRs (Lepp & McCray 1983) respond to the external radiation field by exciting vibrational levels of molecular hydrogen H_2^* . The presence of H_2^* enhances molecular formation (Sternberg & Dalgarno 1995) and it gives rise to a many-lined infrared emission spectrum. The spectrum offers a powerful diagnostic probe of the nature of the incident radiation field and a reliable measure of its intensity. Other strong atomic and molecular emission lines at infrared and microwave frequencies are produced which provide additional probes of the regions (Tielens & Hollenbach 1985, van Dishoeck & Black 1988, Sternberg & Dalgarno 1989, Hollenbach, Takahashi & Tielens 1991, Escalante, Sternberg & Dalgarno 1991, Meixner & Tielens 1993, 1995, Natta, Walmsley & Tielens 1994).

2. Chemistry in dense PDRs

The physical and chemical properties of PDRs are controlled by the incident photons which penetrate the clouds, heat the gas and drive the cloud chemistry. The cloud structure depends on the gas density and pressure, the intensity of the far ultraviolet radiation field, the absorption and scattering properties of the dust grains, the element abundances and the cloud geometry (Tielens & Hollenbach 1985, van Dishoeck & Black 1988, Le Bourlot et al. 1993, Köster et al. 1994, Störzer, Stutzki & Sternberg 1995). In dense clouds which fully absorb the incident radiation, the size of the PDRs is set by the dust opacity to cloud depths corresponding to visual extinctions A_V of a few magnitudes. Detailed model calculations (Sternberg & Dalgarno 1995, Jansen et al. 1995) show that in a PDR photoionization and charge transfer processes give rise to a layered ionization structure. Fig. 1 illustrates the structure for a cloud of density $2 \times 10^5 \text{ cm}^{-3}$. Beyond the H/H_2 transition region which lies adjacent to the ultraviolet source is a zone in which C^+ is the major ion. The molecular ions HCO^+ , H_3O^+ and H_3^+ take over in the dark core where cosmic rays are the principal ionizing agent. For a density of $1 \times 10^6 \text{ cm}^{-3}$ and a radiation field intensity 2×10^5 times

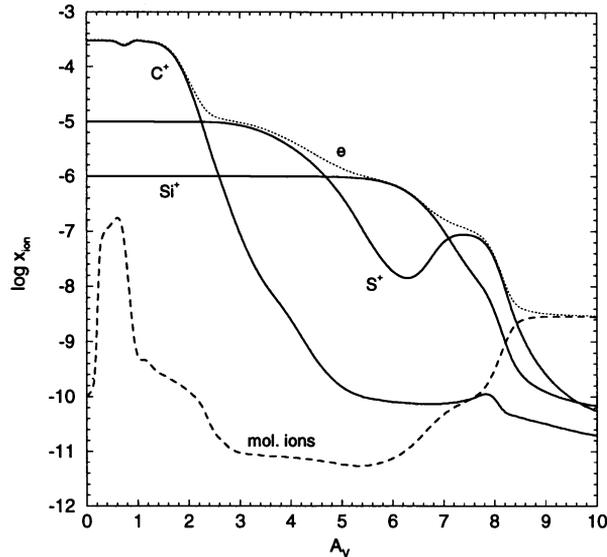


Figure 1. The ionization structure of a photon-dominated region

the mean interstellar value, the S^+ zone begins at a visual magnitude A_V of 2 and the Si^+ at A_V between 4 and 5. The dark core begins at an A_V near 8 mag. Ambipolar diffusion rates and magnetically controlled collapse times are sensitively dependent on the fractional ionization in the different cloud layers (McKee 1989, Hartquist et al. 1993).

In the transition from the C^+ zone to the S^+ zone, C^+ is converted by ion-molecule reactions to CO and to CH. Photodissociation then enhances the abundance of neutral carbon atoms. PDRs at the surfaces of molecular cloud clumps may explain the observed high C/CO ratios as the dissociating ultraviolet radiation penetrates the interclump gas (Phillips & Huggins 1981, Keene et al. 1985, Stutzki et al. 1988, Genzel et al. 1988, Zmuidzinas et al. 1988, Schilke et al. 1993, Tauber et al. 1995). A high fractional abundance of neutral carbon atoms can also be created by recombination of C^+ ions in a cooling ionized region that is shadowed by a cloud (Störzer, Stutzki & Sternberg 1996).

2.1. OH, CO^+ , AND SO^+

In dense clouds with hydrogen nuclei densities n_H greater than 10^3 cm^{-3} the outer edges are hot with temperatures in excess of 10^3 . The gas cools rapidly as atomic hydrogen is converted to H_2 . Once some H_2 has formed, OH is readily produced by the reactions



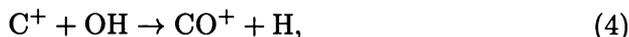
and



The hydroxyl radical is removed by photodissociation



and by the reverse of reaction (1). Large fractional abundances of OH can be achieved. In a cloud with $n_{\text{H}} = 10^6 \text{ cm}^{-3}$ and an ultraviolet radiation field a factor of 2×10^5 more intense than the mean interstellar field the peak OH fractional abundance is 10^{-6} . The OH reacts with the atoms and ions produced by photodissociation and photoionization. The molecular ions CO^+ , SO^+ and SiO^+ are formed by



and



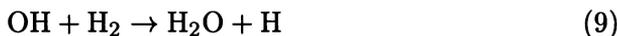
and removed by dissociative recombination, photodissociation and reactions with H_2 . Neutral molecules O_2 and NO are formed by



and



and removed by photodissociation. Water is produced by



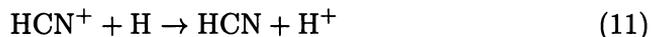
and lost by the reverse reaction to (9) and by photodissociation.

The molecular ion CO^+ attains a fractional abundance of 10^{-9} in the H/H_2 transition layer and disappears at greater depths. Observational evidence for the production of CO^+ in hot PDRs has been obtained by the detection of rotational emission lines of CO^+ at 236.06 and 235.79 GHz in the planetary nebula NGC 7027 and the molecular cloud interfaces in the Orion Bar and M17 (Latter, Walker & Maloney 1995, Störzer, Stutzki & Sternberg 1995). The observations indicate that the emissions peak at the edges of the molecular clouds near but outside the ionization fronts, decreasing sharply in intensity with depth into the clouds (Störzer et al. 1995). The measured line intensities indicate a column density of CO^+ of nearly 10^{13} cm^{-2} , an order of magnitude larger than the theoretical prediction for a PDR. The Orion Bar and M17 are edge-on systems and the optically thin emission may be enhanced by limb brightening.

The ion CO^+ is also produced in dissociative shocks (Neufeld & Dalgarno 1989) so that its presence alone does not establish a PDR as its origin. Dissociative shocks and PDRs may be distinguished by observations of SO^+ and SO . SO^+ has been detected in many astrophysical sources (Turner 1992, 1994). It is produced in dissociative shocks (Neufeld & Dalgarno 1989) and Turner (1992, 1994) has argued that the presence of SO^+ in shocked gas is strong evidence that the shock is dissociative. It is also produced in PDRs. The fractional abundance of SO^+ in the H/H_2 transition zone is 7×10^{-10} in the model of Sternberg & Dalgarno (1995) and a column density of $5 \times 10^{11} \text{ cm}^{-2}$ is predicted for a sulfur fractional abundance of 10^{-5} . The same model predicts a low abundance of SO in contrast to the dissociative shock models in which SO and SO^+ have comparable abundances (Neufeld & Dalgarno 1989).

2.2. CN/HCN DENSITY RATIOS

Another diagnostic probe of PDRs is the CN/HCN density ratio (Fuente et al. 1993, Sternberg & Dalgarno 1995). HCN is created by the reactions



with varying efficiencies in the different zones of PDRs. Its photodissociation



is a major source of CN. Fig. 2 presents calculations of the equilibrium CN/HCN density ratio for PDRs of densities n_{H} greater than or equal to 10^3 cm^{-3} subjected to a radiation field intensity of 2×10^5 times the interstellar value. Fuente et al. (1993, 1995) found enhanced CN/HCN ratios in the reflection nebulae NGC 7023 and NGC 2023. The observed ratios decreased sharply by a factor of seven in NGC 7023 and twenty-five in NGC 2023 with increasing distances from the illuminating stars. In NGC 2023, high density CN filaments coincide in position with infrared emission from vibrationally excited H_2 .

2.3. CS IN NEUTRAL SULFUR ZONES

The CS molecule is often employed as a diagnostic probe of dense gas. It may also be a probe of molecular clouds, illuminated by far ultraviolet

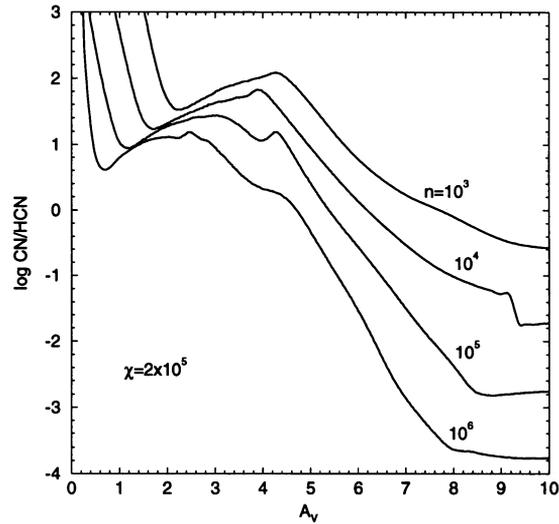
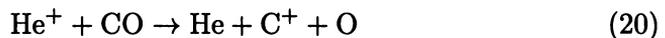


Figure 2. The CN/HCN abundance ratio in a PDR with densities n_{H} greater than or equal to 10^3 cm^{-3} .

radiation. Models (Sternberg & Dalgarno 1995) show an enhancement of CS in the neutral sulfur zone at intermediate cloud depths compared to fully shielded regions. Some S^+ exists in the S I zone and the sequence



produces CS. The S^+ ions and carbon atoms are the result of the cosmic ray ionization of helium, followed by



and



The CS molecules are removed by photodissociation. The peak in the CS density occurs at the inner edge of the S I zone where the far ultraviolet field is attenuated but most of the sulfur is in atomic form. At larger depths, the density of S atoms decreases as sulfur is incorporated into SO and SO_2 .

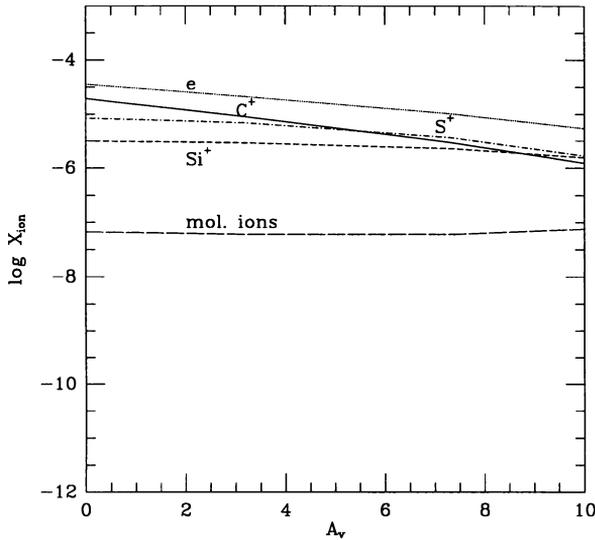


Figure 3. The ionization structure of an X-ray dominated region

In the model of Sternberg & Dalgarno (1995) the CS density is a factor of 10^3 larger at the inner edge of the S I zone than in the dark molecular core.

3. Chemistry of XDRs

The molecular composition of XDRs depends on the intensity of the incident X-rays. Initially, the increased ionization rate accelerates the formation of molecules and molecular abundances are enhanced (Krolik & Kallman 1983) but ultimately the destructive influence of the X-rays dominates (Lepp & Dalgarno 1996). In Fig. 3 we present the ionization structure of an XDR in which the unattenuated ionization rate is $2.5 \times 10^{-13} \text{ s}^{-1}$ and the density is $2 \times 10^5 \text{ cm}^{-3}$. The ionization is dominated by H^+ and He^+ . The chemistry follows the formation and destruction of molecular hydrogen. In the warm zone, the chemistry of hydrogen is similar to that prevailing in the early Universe. Molecular hydrogen is produced by radiative association



followed by



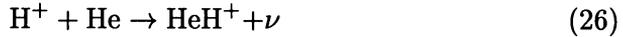
and radiative attachment



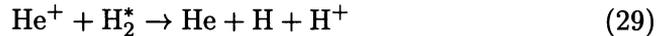
followed by associative detachment



The presence of helium enhances the formation of H_2 through the sequence



and reaction (23). The presence of HeH^+ is a potential diagnostic (Roberge & Dalgarno 1982, Maloney, Hollenbach & Tielens 1996). The H_2 may be vibrationally excited, in which case it can be removed by charge transfer with He^+



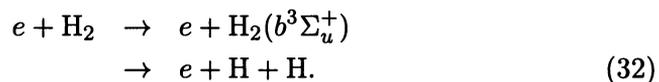
and by dissociative attachment



In the cold zone, H_2 is formed primarily by surface catalysis. It is destroyed in the warm zone by collisional dissociation in neutral particle collisions,



and by electron impact excitation to the dissociative $b^3\Sigma_u^+$ state,



The abundance of H_2 is reduced also through photoionization by photons emitted following radiative recombination of He^+ ions

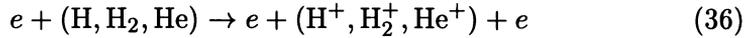


and following excitation of electronic states of He



In XDRs the high frequency X-rays are preferentially absorbed by heavy elements, as in the interstellar gas in inner shell transitions (Morrison & McCammon 1983). The ejection of the innershell electrons is followed by Auger

and radiative Auger decay processes leading to the creation of multiply-charged ions (Weisheit & Dalgarno 1972, Weisheit 1974). The ionization of the light elements H, H₂ and He arises from collisions of the energetic photoelectrons



but the light elements remain partly neutral beyond the fully-ionized zone that lies close to the ionizing source (Lepp & McCray 1983). Neutral hydrogen and helium and multiply-charged heavy ions co-exist. The multiply-charged ions undergo sequential charge transfer. Most are quickly reduced to singly charged ions which enter a chemistry much like that driven by cosmic ray ionization. For some doubly-charged ions, charge transfer may be slow. The doubly-charged ions C²⁺ and S²⁺ may be signatures of XDRs or they may react with H₂ producing CH⁺ (Dalgarno 1976, Langer 1978) and SH⁺.

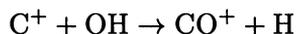
Photodissociation of molecules by ultraviolet photons generated internally by the photoelectrons as they slow down in the gas (Prasad & Tarafdar 1983) is an important mechanism for the destruction of molecules, as are reactions with He⁺ and H⁺. The dissociation products may participate in reactions to form other molecules. Diatomic molecules, particularly hydrides, are resistant to destruction and can exist in considerable abundance in the presence of intense X-ray radiation (Lepp & Dalgarno 1996). Detailed models of XDRs have been constructed by Maloney, Hollenbach & Tielens (1996) and by Yan & Dalgarno (1996a).

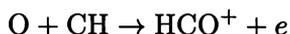
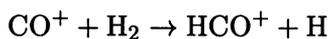
3.1. OH AND H₂O

The chemistry of the X-ray heated zone is similar to that summarized in §2.1. The molecules OH and H₂O are produced in abundance (Lepp & McCray 1983). Neufeld, Maloney & Conger (1994) and Neufeld & Maloney (1995) have argued that water maser emission associated with active galactic nuclei is a result of collisional pumping in dense gas heated by the absorption of X-rays.

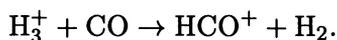
3.2. HCO⁺

The production of HCO⁺ in gas irradiated by X-rays has been discussed by Wolfire & Königl (1993) in a model of the emission from Herbig-Haro objects and by Lepp & Dalgarno (1996) and Yan & Dalgarno (1996b) in a model of the molecular cloud that may surround the hard X-ray source 1E 1740.7–2942. The HCO⁺ is produced in the warm zone by the reactions





and deeper into the cloud by



Phillips & Lazio (1995) carried out interferometric observations of HCO^+ and found that the emission peak is displaced from the source. They attributed the offset to the enhanced destruction and reduced formation of HCO^+ close to the source.

4. Infrared emission of H_2

A powerful diagnostic probe of PDRs and XDRs is provided by the infrared emission from rovibrational levels of molecular hydrogen. Ultraviolet photons are absorbed into the excited ($B^1\Sigma_u^+$) and ($C^1\Pi_u$) states which cascade into the rovibrational levels of the ground state (Gould & Harwit 1963, Black & Dalgarno 1976). The resulting infrared and visible spectra have been calculated in considerable detail (Black & Dalgarno 1976, Black & van Dishoeck 1987, Sternberg 1988, Sternberg & Dalgarno 1989, Draine & Bertoldi 1996, Neufeld & Spaans 1996). Particularly clear examples of PDRs are the reflection nebula NGC 2023 (Gatley et al. 1987, Hasegawa et al. 1987, Burton et al. 1992, Field et al. 1994) and the planetary nebulae Parsamyan 18 (Sellgren 1986) and Hubble 12 (Dinerstein et al. 1988, Ramsay et al. 1993).

In XDRs, the rovibrational levels are populated by cascading from electronically excited states of H_2 arising from photoelectron impact and by rovibrational excitation in direct photoelectron impacts on the lowest $v=0$ vibrational level. The resulting spectrum in a diffuse gas has been calculated by Gredel & Dalgarno (1995) and in a dense gas by Tiné et al. (1996). However, there is no astronomical object in which X-ray pumping has been clearly identified as the excitation mechanism.

5. Time-dependent PDRs

Several recent theoretical studies have addressed time dependent effects in evolving H/H_2 dissociation fronts in PDRs (Goldshmidt & Sternberg 1995; Hollenbach & Natta 1995; Bertoldi & Draine 1996). These studies are motivated by the fact that the equilibrium timescales for the development of H/H_2 photodissociation fronts are often long ($5 \times 10^8/n_{\text{H}}$ yr) compared to the turn-on times ($\sim 10^5$ yr for OB stars, or $\lesssim 10^3$ yr in planetary nebulae) or lifetimes ($\lesssim 10^7$ yr for OB stars, or $\lesssim 10^5$ yr in planetary nebulae) of the

FUV radiation sources. In clumpy clouds in star-forming regions, or in the vicinity of active galactic nuclei fresh material may suddenly be exposed to intense FUV radiation fields as embedded clumps move out from within "shadowed" regions.

Goldshmidt & Sternberg (1995) presented explicit computations and analysis of the time-varying intensities of infrared FUV-pumped fluorescent H₂ emission in (low-density) PDRs. They showed that in clouds exposed to intense radiation fields the H₂ emission line intensities at early times in the evolution of the PDRs are much larger than the line intensities that are produced after the H/H₂ photodissociation fronts reach their equilibrium configurations. In clouds exposed to intense fields the increasing dust opacity associated with the large H I zones that form as the H/H₂ dissociation fronts advance into the clouds reduces the fraction of the incident FUV photons that are absorbed by the H₂ molecules and converted into infrared vibrational emission.

This time-dependent behavior probably explains the unusually intense H₂ line emission observed in several young planetary nebulae. For example, the average surface brightness of the 2.12 μm 1-0 S(1) H₂ line (10⁻³ ergs s⁻¹ cm⁻² sr⁻¹) in the planetary nebula BD+30°3639 is more than 100 times brighter than would be expected under conditions of equilibrium given the observed FUV fluxes ($\chi = 2 \times 10^4$) and densities ($n \lesssim 3 \times 10^4$ cm⁻³) at the edges of the molecular shells. However, this planetary nebula is probably only 10³ yrs old (as inferred from its size and expansion velocity). At this time the predicted H₂ intensity is (for the above values of χ and n) about 100 times larger than the equilibrium value.

Acknowledgements

The work of AD and MY was supported by the National Science Foundation, Division of Astronomical Sciences, under grant AST 95-31790.

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Discussion

Greenberg: Couldn't NH form by reactions on grain surfaces? For typical UV radiation fields, I believe that the dust temperature must be about 70 K. Does this high dust temperature help or hinder?

Dalgarno: Grain surface reactions could be a source of NH. It is usually argued that for diffuse clouds they are such a source. I do not know how they might be modified by a temperature of 70 K.

Fuente: Just a comment. We have detected CO⁺ toward the reflection nebula NGC 7023. The results are shown in a poster.

