ENHANCED OH IN C-TYPE SHOCK WAVES IN MOLECULAR CLOUDS

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Received 1999 August 16; accepted 1999 September 2; published 1999 October 7

ABSTRACT

Cosmic-ray and X-ray ionizations in molecular gas produce a weak far-ultraviolet flux through the radiative decay of H$_2$ molecules that have been excited by collisions with energetic electrons (the Prasad-Tarafdar mechanism). I consider the effect of this dissociating flux on the oxygen chemistry in C-type shocks. Typically, a few percent of the water molecules produced within the shock front are dissociated before the gas has cooled to 50 K. The resulting column density of warm OH rises from $10^{15}$ to $10^{16}$ cm$^{-2}$ as the ionization rate is increased from $10^{-17}$ s$^{-1}$ (typical of dark clouds) to $10^{-15}$ s$^{-1}$ (adjacent to supernova remnants). These column densities produce substantial emission in the far-infrared rotational transitions of OH and are consistent with the OH/H$_2$O ratios inferred from Infrared Space Observatory observations of emission from molecular shocks. For high ionization rates, the column of warm OH is sufficient to explain the OH(1720 MHz) masers that occur where molecular clouds are being shocked by supernova remnants. The predicted abundance of OH throughout the shock front will enable C-type shocks to be examined with high spectral resolution through radio observations of the four hyperfine ground-state transitions of OH at 18 cm and heterodyne measurements of emission in the far-infrared (e.g., from the Stratospheric Observatory for Infrared Astronomy).

Subject headings: ISM: molecules — masers — MHD — molecular processes — shock waves — supernova remnants

1. INTRODUCTION

The energetic electrons produced by cosmic-ray and X-ray ionizations in molecular clouds collisionally excite the Lyman and Werner bands of H$_2$. The subsequent radiative de-excitations generate a weak flux of far-ultraviolet (FUV) photons capable of dissociating many molecular species (Prasad & Tarafdar 1983). Models of chemistry in C-type shock waves have neglected the internally generated FUV photons, which are able to dissociate $\geq 1\%$ of each shock-produced molecular species before the gas cools to 50 K. Although this does not significantly modify the abundances of the parent species, the relatively small abundance of a dissociation product may be of interest. A particularly important example is the dissociation of water to form OH. It is well-established that H$_2$O is formed efficiently from O$^+$ in the hotter part of the shock front by endothermic reactions once $T \approx 400$ K (Draine, Roberge, & Dalgarno 1983; Kaufman & Neufeld 1996). The dissociation of a percent of the water implies an OH abundance of $\sim 10^{-6}$ and column densities $\sim 10^{15}$ cm$^{-2}$.

This column of warm OH is sufficient to explain the high OH/H$_2$O abundances inferred from the Infrared Space Observatory observations of shocked molecular gas associated with the HH 54 outflow (Liseau et al. 1996) and the supernova remnant 3C 391 (Reach & Rho 1998). Enhanced OH abundances associated with shock waves have also been detected at radio wavelengths. OH(1720 MHz) masers are found where supernova remnants are running into molecular clouds (Frail, Goss, & Slysh 1994; Yusef-Zadeh, Uchida, & Roberts 1995; Frail et al. 1996; Green et al. 1997; Koralesky et al. 1998; Yusef-Zadeh et al. 1999a, 1999b). Population inversion occurs by collisions in warm (40–125 K), moderately dense ($\sim 10^3$ cm$^{-3}$) molecular gas in the absence of a significant far-infrared radiation field. In addition, a line-of-sight OH column density between $10^{16}$ and $10^{17}$ cm$^{-2}$ is required for masing to occur (Elitzur 1976; Pavlakis & Kylafis 1996; Lockett, Gauthier, & Elitzur 1999). The conditions for masing in this transition are most likely attained in the cooling tail of a C-type shock wave driven into the cloud by the overpressure within the remnant (Wardle, Yusef-Zadeh, & Geballe 1998, 1999; Lockett et al. 1999), provided that sufficient water can be dissociated in the shocked gas before it cools below $\sim 50$ K.

In this Letter, I present models of the oxygen chemistry in C shocks that include dissociations by internally generated FUV photons. In § 2, I outline the physical and chemical processes that are included in the calculations; results for ionization rates typical of dark clouds and clouds adjacent to supernova remnants are presented in § 3. Warm OH column densities in the range of $10^{15}$–$10^{16}$ cm$^{-2}$ are produced, consistent with the presence of OH(1720 MHz) masers if the shock front harboring the masers is propagating roughly perpendicular to the line of sight—as is expected because the masing cloud should have a small line-of-sight velocity gradient. The implications of these results are briefly discussed in § 4.

2. SHOCK MODELS

The shock structure is assumed to be steady and plane-parallel, with the magnetic field perpendicular to the shock normal. The medium is comprised of neutral and ionized fluids, with the magnetic field frozen into the ionized component and the ionized and neutral components coupled by elastic collisions. The ionization fraction is low, so the inertia and thermal pressure of the ionized component are neglected.

I follow Kaufman & Neufeld (1996) by writing the magnitude of the drag force per unit volume on the neutrals due to the drift of the charged species as

$$F = \left(\frac{\rho}{\rho_i}\right) \frac{\rho_i v_i^2}{L}, \quad (1)$$

where $\rho$ and $\rho_i$ are the densities of the ion and neutral components, $\rho_i$ is the preshock value of $\rho_i$, and $v_i$ is the ion-neutral drift speed. The drag force is in the direction of the ion drift through the neutrals, and there is an equal and opposite force
per unit volume exerted on the ions by the neutrals. The coupling length scale $L$ is determined by the detailed composition of the ionized fluid, which is a mixture of molecular and metal ions, electrons, and charged grains. The calculation of the upstream ionization balance by Kaufman & Neufeld (1996) yields $L \approx 10^{17} (n_\text{H}/10^4 \text{ cm}^{-3})$ cm for the densities of interest here.

The ionization rate $\xi$ is generally assumed to be due to cosmic rays, but X-rays affect molecular gas similarly (e.g., Maloney, Hollenbach, & Tielens 1996), so both ionization sources are notionally lumped together here. The cosmic-ray and X-ray ionization rates depend on the environment: in dark clouds, the standard interstellar cosmic-ray flux yields $\xi \sim 10^{-17} \text{ s}^{-1}$, whereas in molecular gas adjacent to supernova remnants, $\xi \sim 10^{-15} \text{ s}^{-1}$. For example, for a remnant characterized by $L_x = 10^{56} \text{ erg s}^{-1}$ and a radius of 10 pc, $\xi \sim 3 \times 10^{-16} \text{ s}^{-1}$ (see § 4). The cosmic-ray ionization rate may also be of this order if the low-energy cosmic-ray flux is increased by a factor of 100 over the local interstellar value, which seems to be the case for GeV cosmic rays (Esposito et al. 1996). I therefore consider ionization rates in the range from $10^{-17}$ to $10^{-15} \text{ s}^{-1}$.

The ambipolar diffusion heating rate per unit volume, neglecting the heat capacity and radiative cooling by the ionized fluid, is $F_{\text{PDV}}$ by PDV work and by ionizations are also included. Cooling is assumed to occur by collisional dissociation and vibrational transitions of H$_2$ (Lepp & Shull 1983) and by rotational transitions of H$_2$, H$_2$O, and CO (Neufeld & Kaufman 1993; Neufeld, Lepp, & Melnick 1995).

The shock models include a simple reaction network that is sufficient to follow the oxygen chemistry:

\begin{align*}
  \text{H}_2 + \text{H}_2 & \rightarrow \text{H} + \text{H} + \text{H}_2, \\
  \text{O} + \text{H}_2 & \rightarrow \text{OH} + \text{H}, \\
  \text{OH} + \text{H}_2 & \rightarrow \text{H}_2\text{O} + \text{H}, \\
  \text{OH} + \text{OH} & \rightarrow \text{H}_2\text{O} + \text{O}, \\
  \text{OH} + \text{O} & \rightarrow \text{O}_2 + \text{H}, \\
  \text{H}_2\text{O} + \text{FUV} & \rightarrow \text{OH} + \text{H}, \\
  \text{OH} + \text{FUV} & \rightarrow \text{O} + \text{H}, \\
  \text{O}_2 + \text{FUV} & \rightarrow \text{O} + \text{O}. 
\end{align*}

Rates for collisional dissociation of H$_2$ were obtained from Lepp & Shull (1983), and vibrationally cold rate coefficients for reactions (3)–(6) were taken from Wagner & Graff (1987), apart from their forward rate for reaction (5), which is ill-behaved below 300 K—the rate coefficient from the RATE95 database (Millar, Farquhar, & Willacy 1997) is adopted instead. Photodissociation rates for H$_2$, OH, and O$_2$ by internally generated FUV photons were obtained from Grebel et al. (1989).

I adopt shock parameters that are consistent with the OH(1720 MHz) observations toward W28, W44, and IC 443, which imply postshock densities of $\sim 10^3 \text{ cm}^{-3}$ and Zeeman field strengths of $\sim 0.3 \text{ mG}$ (Claussen et al. 1997): a shock speed of $25 \text{ km s}^{-1}$, a preshock density of $n_\text{H} = 10^4 \text{ cm}^{-3}$, and a preshock magnetic field strength of $100 \mu \text{G}$.

3. RESULTS

The shock structure for an ionization rate of $\xi = 10^{-17} \text{ s}^{-1}$, which is typical of cosmic-ray ionization in molecular clouds, is presented in the top panel of Figure 1. The velocities are plotted in the shock frame, in which the shock is stationary, with the unshocked gas flowing in from $z < 0$ at the shock speed (i.e., $25 \text{ km s}^{-1}$), being accelerated within the shock front and departing downstream toward $z > 0$. The middle panel shows the chemical abundances obtained when dissociations by internally generated FUV photons are neglected. As has been found previously (Draine et al. 1983; Kaufman & Neufeld 1996), the preshock atomic oxygen is almost entirely incorporated into water, with OH appearing briefly as an intermediate step. For comparison, the bottom panel shows the effect of including dissociations by internally generated FUV. The overall chemistry is not drastically affected, but the dissociation of water produces an increasing abundance of OH downstream, with a significant column having accumulated by the time the gas has cooled to 50 K. Note also the gradual reappearance of O$_1$ downstream through the dissociation of OH and O$_2$.

The effect of raising the ionization rate to $3 \times 10^{-16} \text{ s}^{-1}$, as
produced by X-rays in a molecular cloud adjacent to a supernova remnant, is illustrated in Figure 2. The ionization fraction of the preshock gas is increased by a factor of $\sqrt{30}$, reducing the thickness of the shock transition and the timescale for gas to flow through the shock front by the same factor. The peak neutral temperature increases because the energy dissipated in the shock must be radiated away on a shorter timescale. Heating associated with ionizations, which is unimportant within the shock front, increases 30-fold, and so the final postshock temperature increases slightly. The photodissociation rate is increased 30-fold, with a concomitant increase in the production of $\text{OH}$ and $\text{O}_2$.

In Figure 3, I summarize the production of OH within the shock models by plotting the run of OH column density with temperature within the shock front for different ionization rates. An initial “burst” of OH column density is produced as oxygen is rapidly converted to water in the high-temperature portion of the shock front. The column density produced during this phase decreases as the ionization rate is increased because the OH-destroying forward reaction (4) is strongly dependent on temperature, and the temperature within the shock rises more rapidly for high ionization rates because of the increase in the rate of ambipolar diffusion heating. If the FUV dissociation is neglected, no more OH is produced (Fig. 3, dashed lines), otherwise OH starts to be produced once the temperature of the shocked gas has dropped sufficiently so that the forward reaction (4) has slowed sufficiently to permit photodissociations to become effective. For high ionization rates, the increase in the photodissociation rate (proportional to $\zeta$) is partially offset by the decrease in the flow timescale (proportional to $\frac{1}{\zeta}$); thus, $N_{\text{OH}} \propto \zeta^{1/2}$ in the cooling gas.

4. DISCUSSION

The line-of-sight column density of warm OH through a C-type shock is $N_{\text{OH}} \sec \theta$, where $\theta$ is the angle between the shock normal and the line of sight. For $\zeta \approx 10^{-16} \text{ s}^{-1}$ and $\theta \approx 80^\circ$, $N_{\text{OH}}$ is sufficient to permit the formation of OH(1720 MHz) masers; thus, typical X-ray fluxes near supernova remnants are able to produce the warm OH column density necessary for OH(1720 MHz) masers.

Lockett et al. (1999) have argued that the X-ray flux from supernova remnants is $\approx 0.02$ of the level that could produce the OH column density necessary for masing in the 1720 MHz line. This discrepancy can be traced to the conversion from the X-ray energy flux $F_X$ to the ionization rate. Both Wardle et al. (1998) and Lockett et al. (1999) used the conversion $\zeta (\text{s}^{-1}) \approx 3 \times 10^{-14} F_X (\text{ergs} \text{ cm}^{-2} \text{ s}^{-1})$ (Maloney et al. 1996), but this assumes a hard X-ray spectrum appropriate to active galactic nuclei. The softer ($E \approx 1 \text{ keV}$) spectrum from the hot gas in supernova remnants produces many more ionizations per unit X-ray luminosity, since ionizations are dominated by low-energy X-ray photons. In this case, $\zeta \approx N_\text{e} \sigma F_X$, where $N_\text{e} \approx 30 \text{ keV}^{-1}$ is the mean number of primary and secondary electrons produced by the absorption of unit energy, $\sigma \approx 2.6 \times 10^{-22} \text{ cm}^{-2}$ is the photoabsorption cross section per hydrogen nucleus at 1 keV, and $F_X = L_X/4\pi R^2$. With $L_X = 10^{36} \text{ ergs} \text{ s}^{-1}$ and $R = 10 \text{ pc}$, this yields $\zeta \approx 4.6 \times 10^{-16} \text{ s}^{-1}$, provided that the hydrogen column density $N_H \approx 10^{22} \text{ cm}^{-2}$. Note that externally incident UV may make a similar contribution to the OH column density if $A_v$ is not too large (Lockett et al. 1999).

The enhancement of OH described in this Letter permits the structure and kinematics of C-type shock waves to be studied
through the modeling of the excitation of OH within the shock front and through the calculation of emission- and absorption-line profiles. Supernova remnants with associated 1720 MHz masers (Frail et al. 1994, 1996; Yusef-Zadeh et al. 1995, 1996, 1999a, 1999b; Green et al. 1997; Koralesky et al. 1998) are obvious observational targets. At radio wavelengths, the four ground-state transitions at 1612, 1665, 1667, and 1720 MHz can be observed with sub–kilometer per second velocity resolution in absorption against the background continuum from the remnant. For example, W28 shows extended OH absorption around the OH maser positions (Pastchenko & Slysh 1974). The predicted warm OH column density within C-type shocks implies substantial far-infrared emission in low-lying OH rotational transitions. This will, for example, be easily detectable by the GREAT heterodyne spectrometer planned for the Stratospheric Observatory for Infrared Astronomy; this spectrometer will be capable of 0.1 km s$^{-1}$ or better velocity resolution.

I thank Cecilia Ceccarelli, Ewine van Dishoeck, Michael Kaufman, and Mark Wolfe for discussions and Phil Lockett for comments on the manuscript. The Special Research Centre for Theoretical Astrophysics is funded by the Australian Research Council under its Special Research Centres programme.

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