EFFECTS OF NONTHERMAL INTERNAL ENERGY ON POSTSHOCK OXYGEN CHEMISTRY

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ABSTRACT. The internal energy distributions of reactants in shocked interstellar clouds are discussed. Rate coefficients appropriate for the oxygen chemistry of shocks differ significantly from those deduced by simple extrapolation of thermal measurements. A one-fluid MHD shock model examines nonthermal effects for a 10 km s⁻¹ shock propagating through clouds of initial densities of 10 and 10^5 cm⁻³, using oxygen-hydrogen reaction rates that are specific to the vibrational, rotational, and fine structure temperatures of the reactants.

The "temperatures" that describe the vibrational, rotational, and fine structure populations of atoms and molecules in shocked interstellar clouds can be significantly lower than the kinetic temperature of the hot postshock gas due to radiative decay and relatively inefficient rotation-translation and vibration-translation transfer. Polar molecules such as OH and H2O decay rapidly to their lowest rotational and vibrational levels. At low and intermediate densities, only heavy homonuclear molecules such as O2 have thermal internal energy; at high densities H2 rotational and vibrational populations also approach their equilibrium values (c.f. Graff and Dalgarno 1986).

Shock-heated diffuse clouds are considered a possible formation site for CH⁺ (Elitzur and Watson 1978, 1980), but reconciliation of observed OH column densities with those predicted by shock models imposes severe constraints on initial conditions (c.f. Mitchell and Watt 1985). The effects of nonthermal vibration, rotation, and fine structure on important postshock oxygen-hydrogen reactions have been studied in detail (Wagner and Graff 1986). The removal of vibrational energy from endothermic reactions such as

 $0 + H_2 \leftrightarrow 0H + H$ (1,2) $0H + H_2 \leftrightarrow H_2 0 + H$ (3,4)

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decreases the reaction rate coefficients. Cold rotational distributions are found to inhibit reaction (1) but enhance reaction (3). Fine structure distributions have little effect on high temperature reactions with large activation barriers but can be important for reactions dominated by long-range barriers.

A one-fluid MHD shock model has been used to determine the effects of nonthermal internal energy on the postshock evolution of the major oxygen-bearing molecules (Graff and Dalgarno 1986). The results for a 10 km s⁻¹ shock propagating through (a) a diffuse cloud of initial density $n_0=10 \text{ cm}^{-3}$ and (b) a dense cloud of initial density $n_0=10^5 \text{ cm}^{-3}$ are shown in Figure 1. In the diffuse cloud, the nonthermal calculation shows a lower OH abundance due to slower production (reaction 1) and faster destruction (reaction 3). In the dense cloud, nonthermal effects cause a significant suppression of oxygen radicals O and OH in the hot gas. The suppression may have a large effect on the formation of heavy molecules by radical-radical reactions.



Figure 1. Postshock evolution of major oxygen-bearing species following a 10 km s⁻¹ shock through (a) a diffuse cloud, $n_0=10 \text{ cm}^{-3}$, and (b) a dense cloud, $n_0=10^5 \text{ cm}^{-3}$, for nonthermal (solid line) and thermal (dotted line) rate coefficients.

REFERENCES

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