INTERSTELLAR SULFUR CHEMISTRY

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ABSTRACT: This paper summarizes results of a chemical model of SO, CS, and OCS chemistry in dense clouds.

The following results were obtained from a theoretical study of sulfur chemistry in dense interstellar clouds using a large-scale time dependent model[1] of gas-phase chemistry. In the results which follow, $f_x = n(x)/n(H_2) \approx N(X)/N(H_2)$ where $N(X) \equiv$ column abundance of X. Also, q(x) and L(x) will denote net production and loss rates of X.

(a) For the large values $f_{O_2} \approx 5 \times 10^{-5}$ predicted by contemporary models[2,3], the reaction[4] $S + O_2 \rightarrow SO + O$ leads to a large[2] value $f_{SO} = 2 \times 10^{-6}$. Observations[5] indicate $f_{SO} \approx (2\text{-}10) \times 10^{-8}$ in L134 and TMC-1. Consequently, f_{O_2} in dense clouds may be much smaller than predicted.

(b) The large value $f_{SO} \sim 10^{-6}$ for dense clouds predicted by Mitchell, Ginsburg and Kuntz[3] results from the reaction $S + H_3^+ \rightarrow H_2S^+ + H$ (1) in their model. Large H_2S^+ production via reaction (1) leads to correspondingly large HS concentration and large q(SO) through the fast reaction $HS + O \rightarrow SO + H$. Reaction (1) probably does not occur, which is consistent with the lower observed f_{SO}.

(c) Due to activation energy[6], the reaction of CS with O atoms is efficient as a loss mechanism of CS during the early phases of cloud evolution (high temperature), or in hot and oxygen rich sources such as the KL nebula. Reactions of H_3^+, HCO^+, H^+ and C^+ serve merely to recycle CS. Consequently, $L(CS) \sim 4 \times 10^{-15}\ s^{-1}$ in dense clouds ($n(H_2) = 2 \times 10^5\ cm^{-3}$, $T \leq 40K$). On this basis, observed[7] $2 \times 10^{-10} \leq f_{CS} \leq 2 \times 10^{-5}$ for $5 \times 10^4 \leq n(H_2) \leq 2 \times 10^5\ cm^{-3}$ implies $q(CS) = 1.6 \times 10^{-18}\ cm^{-3}\ s^{-1}$ in clouds with $n(H_2) = 2 \times 10^5\ cm^{-3}$ and low temperature.

(d) If sulfur is not abnormally depleted in dense clouds, then the observed abundances of SO, SO_2, H_2S, CS, OCS, H_2CS and SiS suggest that sulfur is mostly atomic in dense clouds, i.e., $f_s \sim 10^{-5}$. This

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value for f_S and the low value for q(CS) deduced above jointly imply that the reaction CH + S → CS + H has an activation energy and that $f_{S^+} \leq 5 \times 10^{-11}$ in order that contributions to q(CS) via reactions of S^+ with CH_n do not lead to CS in excess of observations. q(CS) could, however, be substantially higher if condensations onto grains constitute an effective loss mechanism for CS.

(e) In a gas-phase scheme, the reaction chain $SO \xrightarrow{C^+} CS^+ \xrightarrow{H_2} HCS^+ \xrightarrow{e^-} CS$ is the dominant source of CS in dark clouds. $L(CS) \approx 4 \times 10^{-15}\ s^{-1}$ then implies that $n(SO)/n(CS) \simeq 1.6 \times 10^{-5}/n(C^+)$. Using $n(C^+)$ from our models[2], we obtain n(SO)/n(CS) = 3.4, which agrees well with observed value of 4 in L134 or TMC-1. Although it is tempting to interpret this agreement as evidence in favor of gas-phase chemistry, laboratory measurements of the activation energy in the reaction CH + S → CS + H and deduction of upper bounds on f_{S^+} from observations are needed to confirm this inference.

(f) OCS is also stable against reactions with neutral atoms and radicals in dense clouds. Most ionic reactions serve merely to recycle OCS. Consequently, we assume $L(OCS) \approx 4 \times 10^{-15}\ s^{-1}$. The observations of CS in the absence of OCS in a warm cloud, such as Orion A, implies that q(OCS) << q(CS) in this cloud. This is consistent with low f_e in dense clouds[8] and the reaction $S^- + CO \rightarrow OCS + e^-$ as the major source[9] of OCS. In relatively colder clouds (T ≤ 20K), such as Sgr B2, $N(OCS) \gtrsim N(CS)$ has been reported. This implies that additional sources of OCS become important at very low temperatures. The reaction CO + S → OCS + hν, if it occurs, might provide this additional source.

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