MOLECULAR EVOLUTION IN DENSE CLOUDS

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Molecular abundances were calculated time-dependently using a chemical scheme which was carefully constructed to represent the molecular evolution in dense clouds. All ion-neutral reactions of species containing up to 2 heavy atoms (C, N, O, S and Si) were surveyed and a set of possible reactions was selected from numerous exothermic reactions. As molecules containing 3 to 4 heavy atoms are produced by condensation reactions, the scheme was extended. As a result, 234 species, their 2884 gas-phase reactions, and H recombination on grain surfaces were included in our chemical scheme.

A numerical result based on this chemical scheme is shown in Figure 1. The cloud model is: $\zeta_H/n_H=10^{-23}$ (ζ_H is the cosmic-ray ionization rate of an H atom), T=30K, and all elements are initially atomic and have cosmic abundances. As there are numerous species, Figure 1 is divided into four. Observed molecules which are included in our scheme are produced successfully whether small or large. Most molecules reach their peak abundances at $t_c \sim 10^{15}(10^5/n_H)$ s, when most C atoms have been exhausted in forming molecules (mainly CO), and then attain a steady state at $t_s \sim 2\times10^{16}(10^5/n_H)$ s. These time scales are approximately proportional to $1/\zeta_H^{0.6}$ and $1/\zeta_H$ for t_c and t_s respectively, and are very insensitive to n_H. Since these time scales are comparable to the evolutional time scale of dense clouds, time-dependent models are essential. The C/CO ratio is a good indicator of molecular evolution in dense clouds.

Some molecules, especially radicals such as CH, CN and HCO, are overabundant compared with the observations. This should be due to ignoring the effects of neutral-neutral reactions (because they may have activation energies) and condensation onto grain surfaces. Though these processes as well as ejection of molecules from grain surfaces may influence the molecular abundances, the most important part of molecular evolution in dense clouds should be attributed to the ion chemistry in the gas phase.

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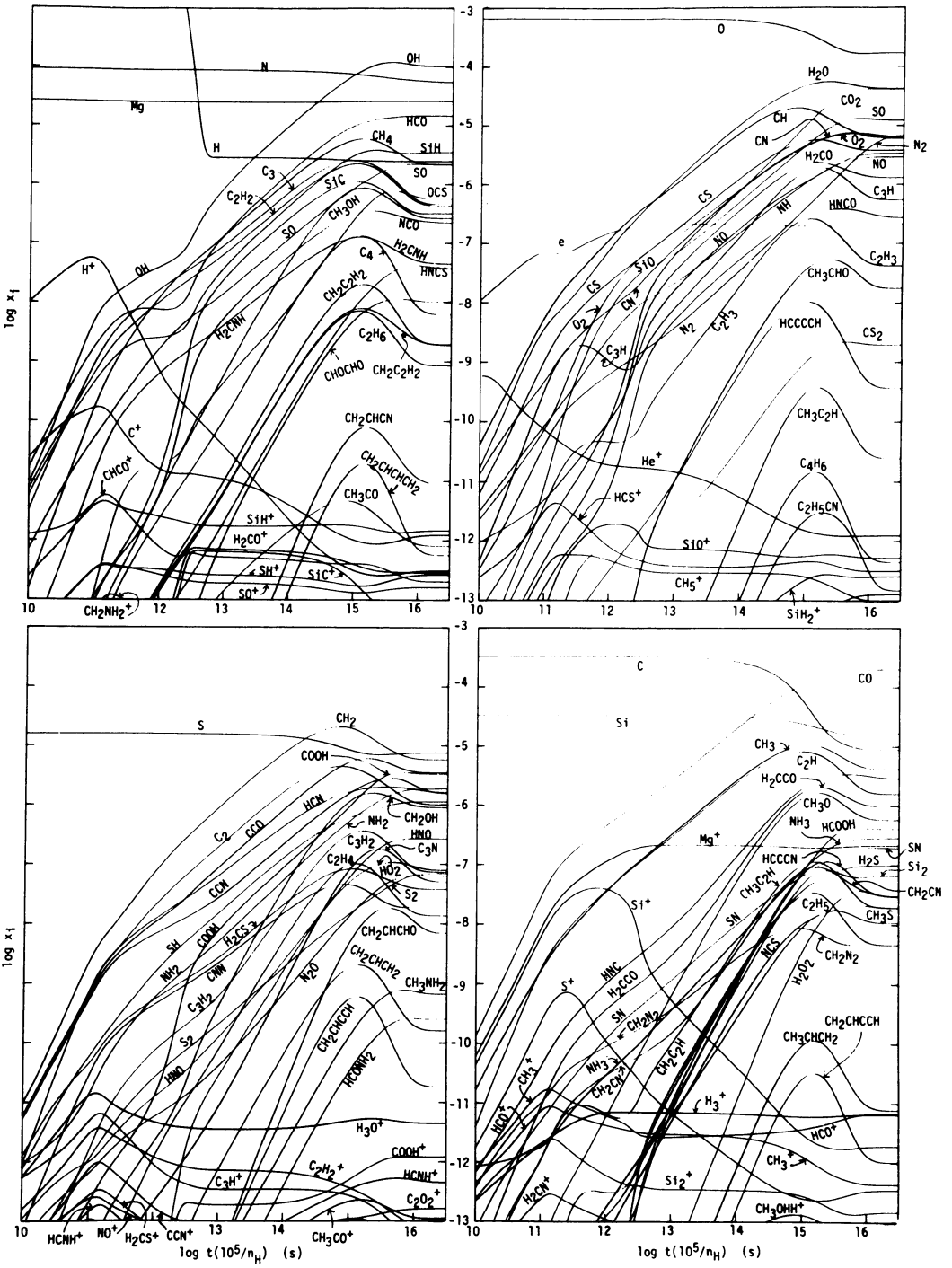

Figure 1. Relative abundances $x_i = n_i / n_H$ versus time t.

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