NUCLEAR SPIN OF H_3^+ AND H_2 IN DENSE MOLECULAR CLOUDS

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The ortho:para ratio of H_2 is a critical parameter for deuterium fractionation in cold, dense quiescent cores. The dominant reservoir for interstellar deuterium is in the inert molecule HD, but the exothermic reaction H_3^+ + HD $\rightarrow$ H_2D^+ + H_2 + 220 K (and H_2D^+ + HD, etc.) can yield highly reactive species capable of distributing deuterium to other molecules. The barrier to the reverse reaction, however, can be overcome even at temperatures below 10 K when ortho-H_2 (o-H_2) reacts with H_2D^+ (or D_2H^+, D_3^+), as ortho-H_2 possesses $\sim$170 K of internal rotational energy in its ground state. Recent modeling work has demonstrated the importance of o-H_2 in cold, dense, highly depleted cores using a chemical network that includes all nuclear spin modifications of H_3^+, H_2, and their isotopologues, but the initial o-H_2 fraction is taken as a parameter in the model. Observationally or computationally constraining this quantity would aid in understanding deuterium fractionation in dense cores.

To learn about the initial o-H_2 fraction in a cold core, we have modeled the chemistry of non-depleted dense interstellar clouds from which cold cores are thought to form. A simplified gas-phase chemical network consisting of 28 species and $\sim$170 reactions is combined with a physical model of a dense cloud, including time-dependent physical conditions. Included in the network are the nuclear spin modifications of H_2, H_2^+, and H_3^+, as well as nuclear spin dependent rate coefficients for the thermalization reactions H_2 + H^+ and H_3^+ + H_2. By modeling the time-dependent chemistry, we find that the ortho:para ratio of H_2 requires 10^7-10^8 years to reach steady state under "standard" dense cloud conditions, which is at least on the order of the cloud lifetime. The timescale depends on the ionization rate, the rate coefficients of the various H_3^+ + H_2 reactions, and the relative abundances of H_3^+ and H^+, but is largely insensitive to the total density and temperature. Even at steady state, the o-H_2 fraction is calculated to be $>$0.5% at 10 K, which is several orders of magnitude above its value at thermodynamic equilibrium. The prospects for using observations of the ortho:para ratio of H_3^+ as a probe of the H_2 ortho:para ratio will be discussed.