SHOCK FORMATION OF INITIAL MOLECULAR ICE MANTLES

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We use a gas-grain chemical network to investigate the initial synthesis of molecular ices as a cold molecular cloud forms behind a shock in the diffuse interstellar medium. The reaction network includes newly measured rates of photodesorption. The results show that CO is first produced in the gas phase in early stages of cloud birth. This is followed by concurrent formation of water ice on the grain and CO accretion to the grain surface from the gas, at intermediate values of the visual extinction. The production of CO_2 occurs on grains, via both diffusive processes and the Eley-Rideal mechanism. The formation of CH_4 ice is inhibited by the gas phase formation of CO. These results show reasonable agreement with detection thresholds for the major ice species, and show best agreement with the observed ice composition along quiescent lines of sight in the Taurus dark cloud for values of A_V of 2-3 mag. When the dense core begins to condense from the cloud, the initial state is not dominated by a gas rich in ionized C, as typically assumed.