Chemistry of Forming Molecular Clouds: Comparison with Molecular Absorption Lines

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Molecular clouds are formed by the compression of atomic gas by interstellar shockwaves. This process is intensively studied using MHD simulations in recent years (e.g. [1]). While these studies include the formation and destruction of major coolants (e.g. O atom, C+, and CO), they do not include less abundant molecules (e.g. carbon-chains) that are observed and used for chemical diagnosis of molecular clouds. So far more than a hundred molecular species are detected in interstellar clouds, and their abundances and spatial distributions are used to investigate the physical conditions and evolutionary stage of clouds.

We aim to fully understand the chemistry in the molecular cloud formation process, including the less abundant molecules for the chemical diagnosis. In the present study, we investigate the chemistry in the shock-compressed layer of $Av \le a$ few mag, which corresponds to diffuse clouds, as a first step. We perform 3D MHD simulations of converging atomic gas flow. We analyze the results to derive the 1D mean flow, along which we solve the detailed chemical reaction network. Compared with previous studies on 1D shock model of cloud formation (e.g. [2], [3]), we cover a wider range of shock parameters such as initial gas density, velocity, and the angle between the gas flow and magnetic field.

We derive the column densities of various species such as HCO+ and C3H2 along the mean flows and compare them with the observations of molecular absorption lines of diffuse clouds observed toward field stars and quasars (e.g. [4]). The column densities vary among the shock parameters, depending on density structures of post-shock regions and timescales of Av. They show reasonable agreement with the observations. We also investigate the dependence of chemistry on cosmic-ray ionization rate, elemental abundance, and PAHs.

References

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