CHEMO-DYNAMICAL MODELING OF CHA-MMS1 TO PREDICT NEW SOLID-PHASE SPECIES FOR DETECTION WITH JWST

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Chemical models and experiments indicate that interstellar dust grains and their ice mantles play an important role in the production of complex organic molecules (COMs). The meeting of chemical species adsorbed from the gas phase onto the grain/ice surface allows reactions to occur efficiently, and leads to the emergence of the ice mantles as a major reservoir of volatile species. To date, the most complex solid-phase molecule detected with certainty in the ISM is methanol (CH_3OH), but it is hoped that the upcoming James Webb Space Telescope (JWST), aided by new laboratory data, will be able to identify yet larger organic species. In this study, we use a coupled chemo-dynamical model to predict new candidate species for JWST detection toward the young star-forming core Cha-MMS1, combining the gas-grain chemical kinetic model MAGICKAL with a 1-D radiative hydrodynamics (RHD) simulation. The abundances of the main ice constituents with respect to water in the model match well with observational values. The model also predicts high solid-phase abundances of intermediate radicals associated with the hydrogenation of CO to methanol (> 0.1 % with respect to water ice). Four oxygen-bearing COMs (ethanol C_2H_5OH, dimethyl ether CH_3OCH_3, methyl formate CH_3OCHO, and acetaldehyde CH_3CHO) as well as formic acid (HCOOH), show abundances as high as > 0.01 % with respect to water ice. N-bearing COMs are generally less abundant than O-bearing ones, suggesting methylamine (CH_3NH_2) as the only N-bearing solid-phase COM candidate for JWST detection.