Progress in Chemical Simulations with Gas and Surface Chemistry

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Astrochemistry is undergoing a period of growth spurred on by a generation of new and more powerful telescopes. Analysis of both current and future data requires, in my view, better and more detailed chemical simulations for diverse sources in both our galaxy and others. A few examples of the need for better simulations will be given. I will then talk about our research program in developing improved gas-grain chemical simulations. The grain surface chemistry will be emphasized because this field of chemistry is still much less certain than gas-phase chemistry for a variety of reasons. Following a history of techniques used to mimic surface/ice chemistry in interstellar sources, I will concentrate on the most detailed stochastic method used to date: the continuous-time random-walk approach [1]. But not only must the chemistry be treated better, the physics must also be improved, and I will discuss our preliminary efforts to develop models including both gas-grain chemistry and 3D magnetohydrodynamics. Initial calculations show that there is a severe problem in the treatment of molecular hydrogen in interstellar ices. A possible resolution of this problem will be discussed [2]. Despite all of these improvements, it may well be that chemical simulations will not be able to keep up with the overwhelming number of data in the ALMA age, and I discuss several alternatives.

References