Rovibrationally-Resolved Reactions for Early Universe Chemistry

P.C. STANCIL, University of Georgia

Investigations of nonequilibrium chemistry in the postrecombination era of the early Universe and in the formation epoch of the first bound structures only consider total collisional reaction rates, i.e., the dependence on the vibrational and/or rotational level of the reactant and/or product molecular species is neglected. In fact, this is the situation for nearly all cases of astrochemical modeling primarily because of the lack of rovibrationally-resolved data. However, recent studies have suggested that the chemistry may be modified, possibly significantly, if vibrational or rovibrational resolution is considered. I will present new quantal calculations for the forward and reverse reactions, $\text{H}^+ + \text{H} \leftrightarrow \text{H}_2^+(v, J) + \nu$, which have considered all 423 bound rovibrational states of $\text{H}_2^+$. The reaction cross sections and rate coefficients display significant variation with $v, J$. The role of these processes in a rovibrationally-resolved chemical model will be illustrated for the evolution of $\text{H}_2^+$ and $\text{H}_2$ in the postrecombination era.

1The work of PCS was supported by NSF grant AST-0087172 and performed in collaboration with A. Dalgarno, J. Green, S. Lepp, and Z. Wang.