The effect of non-equilibrium kinetics on oxygen chemistry in the interstellar medium

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Abstract

The $O+H_2$ →$OH+H$ reaction is considered to be the key step in initiating oxygen chemistry in shocked interstellar molecular clouds. We present extensive quantum scattering calculations of rate coefficients of the $O+H_2 \rightarrow OH+H$ reaction involving both ortho and para hydrogen in the temperature range 100–4000 K. The reaction is slow at low temperatures with ground state reactants due to an energy barrier in the entrance channel of the reaction. The role of non-equilibrium vibrational populations of H_2 is examined and it is shown that vibrational excitation of the molecule has a significant effect on reactivity, especially at low temperatures. At 100 K, the rate coefficient increases by about 11 orders of magnitude when the H_2 vibrational quantum number is increased from $v = 0$ to $v = 3$. Initial vibrational state selected cross sections, rate coefficients as well as product OH vibrational level distributions are presented for $v = 0 - 3$ of the H_2 molecule.

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