A framework for incorporating binding energy distributions in astrochemical models

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One of the most severe limitations of the current astrochemical models is that only a single type of binding site is considered, although laboratory and quantum chemical studies have found that there are multiple types of binding sites with different potential energy depths [e.g., 1, 2]. On a surface with multiple types of binding sites, adsorbed species can be trapped in sites with a deep potential, increasing the resident time of the adsorbed species. On the other hand, species can be populated in shallow potential sites, activating thermal hopping and thus two-body reactions even at low temperatures, where thermal hopping from deeper sites is not activated. Such behavior cannot be described by the conventional rate equation method [3, 4].

I present a framework for incorporating binding energy distributions in gas-ice astrochemical models as a natural extension of the conventional rate equation method. I developed a simple method to estimate the probability distribution function for the occupation of binding sites with different potential energy depths, assuming a quasi-steady state. By using hopping and desorption rates weighted by the probability distribution functions, the effect of binding energy distribution is incorporated into the rate equation method without increasing the number of ordinary differential equations to be solved. This method was found to be accurate and computationally efficient and enables us to consider binding energy distributions even for a large gas-ice chemical network, which contains hundreds of different icy species. The impact of the binding energy distribution on the interstellar chemistry will be discussed quantitatively.

References

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