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Reaction rate measurements between sympathetically cooled ions and velocity selected polar molecules: search for the deuterium isotope effects

Yusuke Takada and Kunihiro Okada[1]

[*] Department of Physics, Sophia University, 7-1 Kioicho, Chiyoda, Tokyo 102-8554, Japan

Synopsis The rates of cold ion-polar molecule reactions are measured at a temperature lower than 10 K in order to search for the deuterium isotope effects.

Cold ion-molecule reactions at a temperature lower than 100 K are very important for astrochemistry [1]. However, there is a wide gap between the temperature required of the reaction rates in astrochemistry and the temperature of the available measurements. Actually most of such measurements were performed at the restricted range near room temperature [2]. In particular cold ion-polar molecule reactions have not been measured extensively at low temperatures owing to experimental difficulties, such as condensation or sublimation of polar gases. Actually the experimental information of the reactions at temperature lower than 77 K is missing. However, recent experimental developments combining a linear Paul trap for generating ion Coulomb crystals with a Stark velocity filter for producing cold polar molecules make it possible to measure the cold ion-polar molecule reactions under ultra-high vacuum conditions [3]. Recently we have demonstrated the reaction rate measurements between the sympathetically cooled N_2H^+ ions and cold CH_3CN molecules using the technique [4]. This potential technique possibly enables to find out quantum effects in cold ion-polar molecule reactions through systematic measurement.

In this work we search for the deuterium isotope effects in cold ion-polar molecule reactions. Up to now we have measured six reactions between cold acetonitrile isotopomers (CH_3CN, CD_3CN) and three sympathetically cooled ions (N_2H^+, N_2D^+ and Ne^+). As mentioned above, velocity-selected acetonitrile molecules were produced by the Stark velocity filter, which was previously described [4]. The translational temperature of about 6.5 K was estimated by combining the result of the time-of-flight measurement to the numerical simulations of the velocity filtering of the molecules. On the one hand, the average ion-kinetic energy, which is mainly determined by the micromotion energy, was evaluated by performing molecular dynamics simulations of two-component ion Coulomb crystals with the similar size as the observed crystals [4, 5]. As a result, the average-reaction temperature in the present reactions was estimated to be lower than 10 K, which corresponds to the energy lower than 1.2 meV. Thus, it is possible to detect the deuterium isotope effect if there is a reaction barrier larger than 1.2 meV in one of the pair of the present reactions.

Figure 1 (a) (b) show examples of the reaction rate measurements between velocity-selected acetonitrile molecules and sympathetically cooled Ne^+ ions. The graphs show plots of relative number of Ne^+ ions embedded in the Ca^+ ion Coulomb crystal as a function of the reaction time. The inset images give signification of LIF images of two-component Coulomb crystals consisting of Ca^+ and Ne^+ ions in the initial conditions of the measurements. We observed a difference in the reaction rates between (a) and (b) reactions. Details of the experiment, discussions and the results of the other reactions will be presented at the conference.

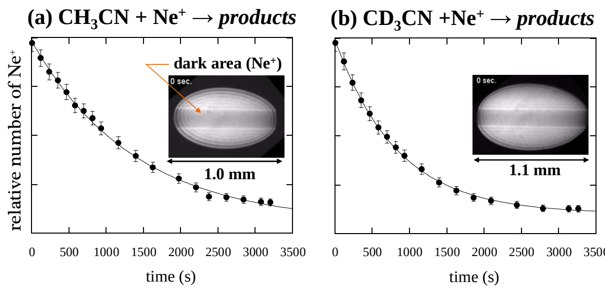

Figure 1. Reaction rate measurements between velocity-selected acetonitrile molecules and sympathetically cooled Ne^+ ions (see text).

References

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[1] E-mail: okada-k@sophia.ac.jp