Quantum-State Resolved Study of the Ultracold K+KRb Reaction

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Synopsis We report a numerically exact quantum mechanical treatment of the K+KRb reaction and discuss both universal and statistical aspects of its reaction dynamics. It is shown that the total rate is universal in character - validating the use of universal models in other similar reactions. However, the rotational distribution is shown to be statistical in character - which we argue is due to the chaotic nature of the reaction complex.

Chemistry's ultimate goal is the absolute control of quantum states of both reactants and products. This is only achievable in the ultracold regime where precise control over initial states including, nuclear spin orientation is possible. In a landmark experiment, research groups at JILA were able to produce an ultracold gas of ^{40}K^{87}Rb molecules at nano Kelvin temperatures where even the nuclear spins were oriented [1]. Rate coefficients for exothermic reactions between KRb+KRb and KRb+K were also reported. It was shown that by merely flipping a nuclear spin the reaction could be turned on and off.

An explicit quantum calculation of reaction dynamics for such systems poses a formidable computational challenge, as the computational costs scale with the cube of the number of channels. For these reasons, while the pioneering experiments [1] on KRb reactions were performed over six years ago, no accompanying scattering calculations have been performed at the state-resolved level, until now [2].

Here, we report explicit quantum calculations of the K+KRb→K_2+Rb reaction with resolution of rotational and vibrational level of the product K_2 molecule. Figure 1 provides a comparison of rate coefficients from the present study along with the experimental result of Ospelkaus et al. [1] and predictions of a universal model. It is seen that the computed results are within a factor of two of the experiment and in excellent agreement with the prediction of the universal model suggesting its validity. The experimental result corresponds to a translational temperature of about 250 nK and only s-wave contributes at this temperature. The figure also shows that the total rate is insensitive to three-body forces in the interaction potential. The vibrationally resolved rates indicate that the reaction populates vibrational levels $v' = 0 - 2$ at comparable rates. The high density of states allows a statistical description of the reaction dynamics. An analysis of the rotational population reveals a Poisson distribution.

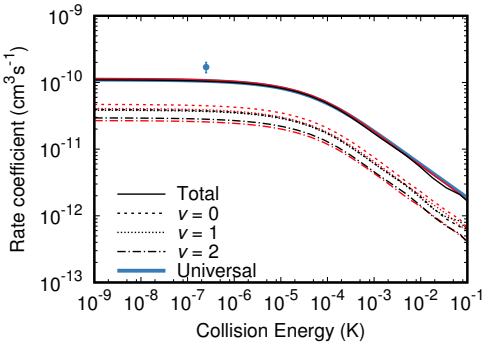

Figure 1. Rate coefficient for K+KRb($v = 0, j = 0$) →$K_2(v')$+Rb reaction as a function of the translational temperature. The red curves are based on a pairwise potential that does not include three-body forces and the black curves are from an interaction potential that includes three-body forces.

References

[1] S. Ospelkaus *et al.* 2010 *Science* **327** 853.

[2] J. F. E. Croft *et al.* 2017 *Nature Comm.* (submitted).

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