Ultracold chemical reactions: from reactants to products

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ABSTRACT

Ultracold molecules can be used to probe chemical reactions with an unprecedented control at the quantum level. All the fragments of an ultracold chemical reaction, from reactants to products, including intermediate complexes, can now be observed by ionization spectroscopy and velocity-map imaging [1]. Molecules possess electronic, vibrational, rotational and spins degrees of freedom and the way they end up in a chemical reaction via the re-arrangement of the atoms is complex. While a full quantum treatment of all degrees of freedom for heavy barrierless systems is for the moment not yet achieved, one can investigate, as a first step, up to which point the nuclear spin degrees of freedom are linked to the remaining ones in a chemical reaction.

A recent study [2] showed that experimental data are consistent with a theoretical model based on the condition that the nuclear spin degrees of freedom mainly act as spectators in chemical reactions of ultracold bi-alkali molecules in magnetic fields. This leads to the possibility to control the rotation parities of the molecular products (even versus odd quantum numbers) with a magnetic field. We further extend this theoretical model and propose a more analytical and general expression for the relative nuclear spin state-to-state distribution of an ultracold chemical reaction in a magnetic field [3]. We show that it simply requires the knowledge of the eigenfunctions of the molecular reactants and products of the chemical reaction in the magnetic field.

We apply our formalism to the KRb + KRb → K_2 + Rb_2 ultracold reaction studied in the group of Harvard [1,2]. We present the relative nuclear spin state-to-state distribution probabilities of the products given an initial quantum state of the reactants as a function of the magnetic field. The magnetic field trend of the summed probabilities is in very good agreement with recent experimental results of the Harvard group [2].

References

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[2] Hu, Liu, Nichols, Zhu, Quéméner, Dulieu, Ni, "Nuclear spin conservation enables state-to-state control of ultracold molecular reactions", arXiv 2005.10820 (2020), accepted to Nature Chemistry

[3] In preparation.