Theoretical study for the exchange reactions of H' + NH → NH' + H and D + NH → ND + H

Xian-Fang Yue* [1]

* Department of Physics and Information Engineering, Jining University, Qufu 273155, China

Synopsis In this work, the author has investigated the rotational integral cross sections and product angular distributions of the title reactions. The results are compared with previous work, and large differences were found and compared.

NH and NH_2 radicals are of great importance in nitrogen chemistry in flames. Therefore, the title reactions have been studied in both experimental [1-2] and theoretical [3-4] aspects. Qu *et al.* [1] measured the rate coefficients of the reaction NH($X^3\Sigma^-$) + D(^2S) in a quasistatic laser-flash photolysis, laser-induced fluorescence system. Li *et al.* [3] carried out the exact quantum mechanical (EQM) and statistical quantum mechanical (SQM) calculations using a quantum wavepacket method. In the present work, the author has carried out the investigation of the title reactions by employing the quasi-classical trajectory (QCT) method.

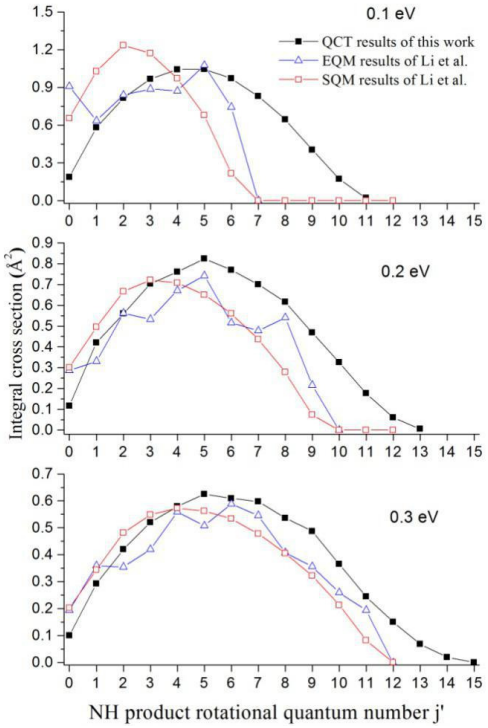


Figure 1. Comparison of the rotational integral cross sections for the H' + NH (v=0, j=0) → NH' (v', j') + H reaction at three collision energies obtained with the QCT method by this work and the EQM and SQM methods by Li *et al.* [3].

As shown in Figure 1, all of the nascent NH product from the reaction H' + NH (v=0, j=0) → NH' (v', j') + H are in the ground vibrational state. However, their rotational state distribution is inverted. These are in consistent with previous EQM and SQM results studied by Li et al. [3]. At the collision energy of 0.1 eV, the ground rotational state distribution of the QCT calculations is lower than that of both the EQM and SQM [3]. This may be due to the quantum effect. At collision energies of the 0.2 and 0.3 eV, the product rotational state distributions of the QCT results are in good agreement with the EQM and SQM [3], meaning that the quantum effect becomes weak in high collision energies.

The product vibrational and rotational state distribution demonstrate that the title reaction via an indirect reaction mechanism. The reaction mechanism is also can be deduced through characters of the differential cross section (DCS). The DCS of the H' + NH (v=0, j=0) → NH' (v', j') + H reaction shows the backward and forward distributions, which indicates that the reaction process undergoes a longer time. That is to say, the title reaction is indirect.

The vector correlations between the product and reactant are also calculated. The results indicate that the product rotational angular momentum $\boldsymbol{j'}$ is not only aligned, but also oriented along the negative direction of *y*-axis.

References

[1] Z.-W. Qu *et al.* 2005 *J. Chem. Phys.* **122** 204313
[2] H. Umemoto et al. 1997 *J. Chem. Phys.* **106** 4985
[3] Z. Li *et al.* 2009 *J. Chem. Phys.* **131** 1243133
[4] S. Y. Lin *et al.* 2006 *Phys. Rev. A.* **74** 022703

[1] E-mail: xfyuejnu@163.com

Content from this work may be used under the terms of the Creative Commons Attribution 3.0 licence. Any further distribution of this work must maintain attribution to the author(s) and the title of the work, journal citation and DOI.
Published under licence by IOP Publishing Ltd