Rotational relaxation in ultracold He+BH collisions*

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Collisions of cold and ultracold BH in the $\nu = 0$ level with the He atom are investigated using the quantum mechanical scattering formulation. The elastic and the inelastic cross sections are calculated using the two-dimensional *ab initio* potential energy surface. It is shown that the elastic cross section is larger than the inelastic one. When the collision energy is very low, the elastic cross section follows the Wigner threshold law and is one order of magnitude larger than that of He–O_2, while it is much smaller than that of He–H_2. The efficiency of the rotationally quenching state is given. The $\Delta j = -1$ transition is most efficient. The resonances are also found to occur at about the same translational energy (0.1–1 cm^{-1}), which gives rise to steps in the rate coefficient at temperatures around 0.1–1 K.

Keywords: He–BH complex, cold collisions, rotation quenching, cross section

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1. Introduction

Currently, many related investigations of the relaxation of rovibrationally excited molecules at very low energy are being carried out because of the strong interest for cooling and trapping atoms and molecules at ultralow temperatures. The ultracold molecules may be useful for the high-resolution molecular spectroscopy and the investigation of reactions at ultralow temperatures. To help design a stable source of molecular condensates, the efficiency of rotational transition for molecules at ultralow temperatures needs to be investigated. During the past years, major developments in this very active field have provided a new probe for fundamental physics. Several experimental approaches, which include the photo association of ultracold atoms, the buffer gas cooling technique and the cooling by using time-varying electric field, have been proposed and realized.[1,2]

Motivated by experimental methods, such as the helium buffer gas cooling and the helium cluster isolation spectroscopy, the theoretical study acts as a helium atom collision partner. For example, the He+CO,[3] He+CaH,[4] He+O_2,[5] and He+H_2^+[6] have been studied. In the previous papers,[7,8] we have studied the two-dimensional intermolecular ground state potential of the He+BH complex and constructed the three-dimensional interaction potential energy surface.

Regardless of the specific experimental scheme, the efficiency of cooling depends on the relative magnitudes of the elastic and the inelastic scattering cross sections. So, it is crucial to theoretically study the elastic and the inelastic scatterings at the very low energy regime. The quantum mechanical effect plays a dominant role at very low temperatures, and the atom–molecule dynamics is very sensitive to the weak intermolecular force between the atoms and the molecules. Considering the structures and the dynamics of BH with rare-gas atom complexes, Wang and Dagdigian[9] reported the LIF spectra for the $A^1\Pi \rightarrow X^1\Sigma$ transition of the Ar–BH complex. Alexander *et al.*[10] calculated the potential energy surface of the Ar–BH ($A^1\Pi$, $X^1\Sigma$) complex using a multi-reference configuration interaction method (MR–CI(D)). In 2009, Wang *et al.*[11] calculated the elastic, the inelastic and the differential cross sections for the collisions between the He atom and the ground state of the BH molecule. However, to our knowledge, there is no report on boron family hydrides colliding with the rare-gas atom complex at very low energy. As a matter of fact, we studied the cross section for the vibrational relaxation of the He+BH complex in 2010 and showed that the inelastic cross sections follow the Wigners law at very low kinetic energy and the $\Delta v = -1$ transition is more efficient than the $\Delta v = -2$ one.[8] In the present work, we carry out the investi-

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gation of the rotational relaxation of the BH in the $v = 0$ level at cold temperatures.

The rest of the present paper is organized as follow. In Section 2, the method and the parameters used for the scattering calculations are briefly discussed. Results and discussion are given in Section 3.

2. Theoretical method

The details of the theoretical method have been given in Refs. [8], [12] and [13]. The coupled-channel Schrödinger equation is solved using the R-matrix method. The cross sections for the transitions from an initial vibrational–rotational level labeled by quantum numbers vj to a final level labeled by quantum numbers $v'j'$ can be expressed in terms of the corresponding S-matrix elements as

$$\begin{aligned}&\sigma_{vj\to v'j'}\\&=\frac{\pi}{2\mu(E-E_{vj})(2j+1)}\sum_{J}^{\infty}(2J+1)\\&\quad\times\sum_{l=|J-j'|}^{|J+j|}\sum_{l'=|J-j'|}^{|J+j'|}\left|\delta_{jj'}\delta_{ll'}\delta_{vv'}-S^{J}_{vjl;v'j'l'}\right|^2,\end{aligned}\quad(1)$$

where J and l are the total and the orbital angular momentum quantum numbers, respectively, $S^J_{vjl;v'j'l'}$ is an element of the S matrix and can be obtained from the solution of the usual close-coupling equations and E_{vj} is the kinetic energy in the initial channel. The rate coefficients are given by

$$\begin{aligned}&R_{vj\to v'j'}(T)\\&=(8k_{\rm B}T/\pi\mu)^{1/2}\frac{1}{(k_{\rm B}T)^2}\\&\quad\times\int_0^{\infty}\sigma_{vj\to v'j'}(E_{\rm K})\exp(-E_{\rm K}/k_{\rm B}T)E_{\rm K}\,{\rm d}E_{\rm K},\end{aligned}\quad(2)$$

where $k_{\rm B}$ is the Boltzmann's constant , T is the temperature and μ is the three-body reduced mass. The total quenching rate coefficients are given by

$$R_{vj}(T)=\sum_{v'j'}R_{vj\to v'j'}(T).\quad(3)$$

Equations (1) and (3) may be used to obtain the components of the complex scattering length, $a_{vj}=\alpha_{vj}-{\rm i}\beta_{vj}$. The imaginary part is determined by ($\hbar$ is the reduced Plank constant)

$$\lim_{T\to 0}R_{vj}(T)=\frac{4\pi\hbar\beta_{vj}}{\mu},\quad(4)$$

and the real part by

$$\sigma_{vj\to v'j'}=4\pi(\alpha^2_{vj}+\beta^2_{vj})\approx 4\pi\alpha^2_{vj},\quad(5)$$

which is the elastic-scattering cross section in the limit of zero energy. In the limit of zero temperature, the Wigner's law holds and the quenching rate coefficients attain finite values.

Based on the CCSD (T) two-dimensional intermolecular ground state potential energy surface of the He–BH complex,[7] we have used a 32-point Gauss–Legendre quadrature to project out the expansion coefficients. The Legendre polynomials require $\lambda_{\rm max}=11$. The cross sections are calculated using the nonreactive molecular scattering program MOLSCAT and computed in the energy range of 10^{-5} cm^{-1} $\leq E\leq$ 10^4 cm^{-1} to evaluate the rate coefficients. The tolerance parameters and the step size are all carefully checked at the selected energies to ensure the convergence of the cross section upon the collision energy.

3. Results and discussion

Figure 1 shows the rotational cross sections of the $j=7$ states of BH. The elastic cross sections are larger than the total inelastic cross sections. As can be seen, the elastic cross section is about 10 times larger than the total inelastic cross section when the kinetic energy is around 10^{-4} cm^{-1} and the former is about 100 times larger than the latter at energy near 0.1 cm^{-1}. This scenario is beneficial to the reduction of the trapping loss and the further cooling by the vapouring means. On the other hand, the rotational quenching cross section for $j=7\to j'=6$ is the largest one and the process determines the total quenching cross section. So the $\Delta j=-1$ transition is the most efficient. We compare the quenching cross sections of $j=5\to j'=4$ with

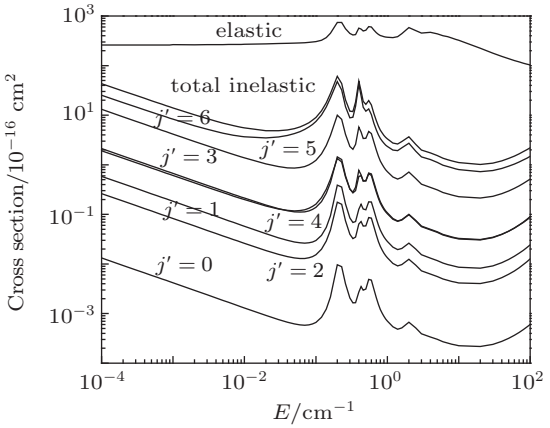


Fig. 1. Rotational cross sections of BH ($j=7$) in collision with ^{3}He versus the kinetic energy.

those of $j = 6, 7 \rightarrow j' = 4$ in Fig. 2. The quenching cross sections decrease with the increase of Δj. The quenching curves in Figs. 1 and 2 have similar structures. Resonances are also found to occur in the translational energy region of 0.1–1 cm^{-1}, which is caused by a centrifugal barrier.

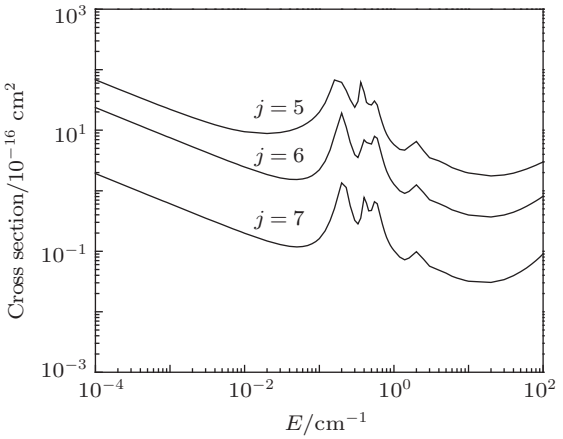


Fig. 2. Quenching cross sections for $j' = 5, 6, 7 \rightarrow j' = 4$ versus the kinetic energy.

The corresponding rate coefficients are presented in Fig. 3. For the $j = 7$ state, the quenching rate coefficient exhibits a maximum around 0.3 K, which is due to the contributions of the shape resonances shown in Fig. 1. When the temperature decreases from 0.3 K to 0.01 K, the quenching rate coefficient presents a drop tendency. As the temperature further decreases, the quenching rate coefficient curve becomes flat and the quenching rate coefficient tends to be a finite value, which accords with the Wigner's law. The corresponding elastic rate coefficient decreases as the temperature reduces and is one order of magnitude larger than the quenching rate coefficient, which is beneficial to cooling and trapping molecules.

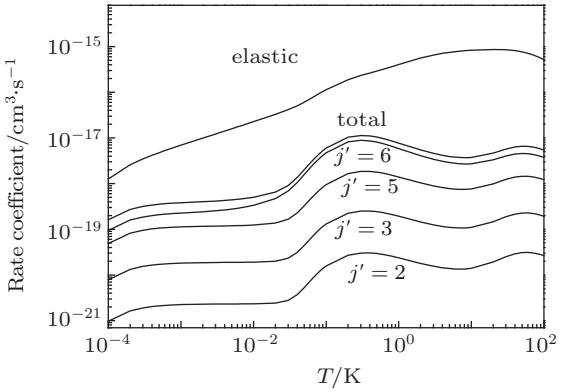


Fig. 3. Rate coefficients of the $j = 7$ level of BH in collision with ^{3}He versus the temperature.

Figure 4 shows the elastic cross sections of BH ($j = 3, 5, 7$) in collision with ^{3}He, each as a function of the kinetic energy. When the kinetic energy is less than 0.01 cm^{-1}, the elastic cross sections tend to be constant values, showing ordinary profiles similar to that of the van der Waals complexes with a very low energy Wigner regime. The constant values are in the order of 10^2 Å. They are 10 times larger than the constant value of He–O_2[5] and are 500 times smaller that of He–H_2,[6] indicating that cooling BH molecule is easier than cooling O_2 but is more difficult than cooling H_2. In Fig. 5, we find that the curves of the elastic rate coefficients of the $j = 2, 4, 6$ levels of BH in collision with ^{3}He are mostly coincident.

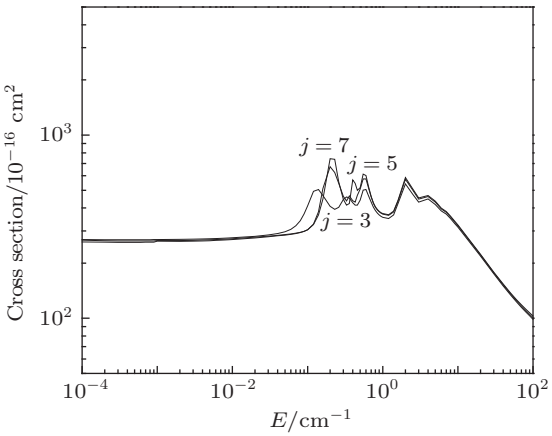


Fig. 4. Elastic cross sections of BH ($j = 3, 5, 7$) in collision with ^{3}He versus the kinetic energy.

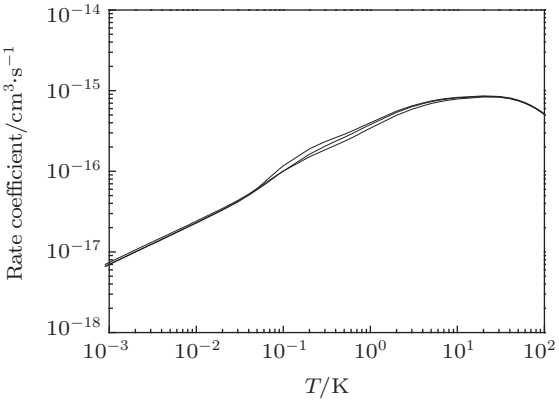


Fig. 5. Elastic rate coefficients of the ($j = 2, 4, 6$) level of BH in collision with ^{3}He versus the temperature.

Further, we compare the ratios of the quenching cross sections to the elastic cross section for different initial levels of BH in Fig. 6. The ratios are less than 0.4 when the kinetic energy is greater than 0.01 cm^{-1}. And the ratio increases as j decreases. The high ratio is not conducible to cooling and trapping molecules.

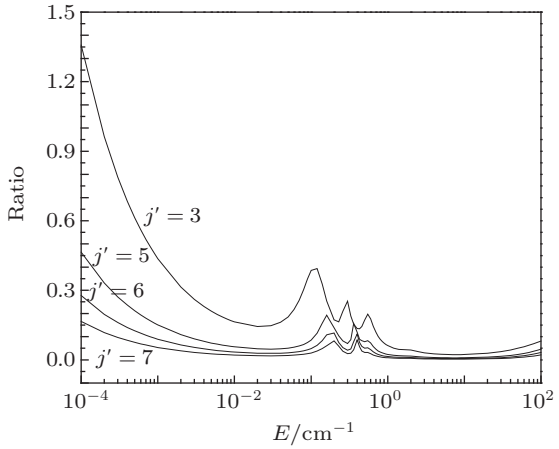


Fig. 6. Ratios of quenching cross sections to elastic cross section versus the kinetic energy.

4. Conclusion

According to the CCSD(T) two-dimensional potential energy surface, we perform the quantum mechanical coupled-channel scattering calculation for the rotational relaxation of the BH in the $\nu = 0$ level in collision with the ultracold He atoms. We calculate the elastic and the inelastic cross sections and the corresponding rate coefficients. We find that the elastic cross sections are larger than the inelastic ones and the $\Delta j = -1$ transition is the most efficient. When the collision energy is very low, the elastic cross sections tend to be constant values and the inelastic cross section increases linearly with the decrease of the collisional velocity, which follows the Wigner threshold law. On the other hand, the elastic cross sections are one order of magnitude higher than those of He–O_2 and much smaller than those of He–H_2. The inelastic cross sections are two orders of magnitude higher than those of He–O_2. They indicate that cooling BH molecular is more difficult than cooling H_2, while it is easier than cooling O_2. We find that the resonances occur at about the translational energy of 0.1–1 cm^{-1} because of the centrifugal barrier, which gives rise to steps in the rate coefficients for temperatures around 0.1–1 K.

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