Vol 16 No 11, November 2007
1009-1963/2007/16(11)/3352-07
Chinese Physics
© 2007 Chin. Phys. Soc.
and IOP Publishing Ltd

Theoretical calculation of the partial cross section for first vibrational excitation in He–H_2(D_2,T_2) collisions*

Shen Guang-Xian(沈光先)[a)b)†], Linghu Rong-Feng(令狐荣锋)[a)b)],
Wang Rong-Kai(汪荣凯)[b)], and Yang Xiang-Dong(杨向东)[a)‡]

[a)] *Institute of Atomic and Molecular Physics, Sichuan University, Chengdu* 610065, *China*

[b)] *School of Sciences, Guizhou Normal University, Guiyang* 550001, *China*

(Received 28 December 2006; revised manuscript received 30 January 2007)

In this paper, close-coupling method was applied to the He–H_2(D_2,T_2) system, and the first vibrational excitation cross sections of '00–10, 00–12, 00–14, 00–16' at different incident energy have been calculated. By analyzing the differences of these partial wave cross sections, this paper have obtained the change rules of the partial wave cross sections with increases of quantum number, and with change of reduced mass of system. Based on the calculation, influence on the partial wave cross sections brought by the variations in the reduced mass of systems and in the relative kinetic energy of incident atoms is discussed.

Keywords: cross section, close-coupling method, isotope
PACC: 3440, 3450

1. Introduction

The inelastic vibrational scattering of an atom by a diatomic molecule is of both theoretical and practical importance. It plays a very important role in practical processes, such as the cooling of interstellar matter, predicting the laser action, resonance fluorescence and gas phase relaxation etc. Moreover, it can serve as a prototype for general molecular collision.

The collision between a helium atom and a hydrogen molecule is one of the simplest molecular scattering systems and it has received much attentions.[1−8] Since hydrogen has three isotopes, the effect of isotopic substitution must be considered. To obtain the magnitude of the isotope effect in practical systems and to determine the accuracy in the measurement which is influenced by this effect, the isotope substitution effect in atom–molecule collision must be realized.[9−11] However, a little has been reported in this field and few data are available.

The rotational and vibrational excitations take place at the same time when the incident energy of atom is higher than the vibrational excitation energy level of target molecule. This course is more complex than that of simplex rotational excitation. Close coupling calculations[12,13] and T–T potential model[14] are employed for scattering between an atom and a diatomic molecule. Inelastic cross sections of simplex rotational excitation for simple system are calculated by using this method previously.[11,15−18] In this paper, theoretical calculations and systematical studies of the cross sections for vibrational and rotational excitation taking place at one time in He–H_2,D_2,T_2 collisions are presented.

2. Calculations of interaction potential in He–H_2(D_2,T_2)

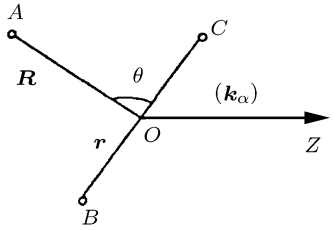


Fig.1. The collision of one atom and diatomic molecule.

*Project supported by the National Natural Science Foundation of China (Grant No 10574096), the Specialized Research Fund for the Doctoral Program of Higher Education of China (Grant No 20020610001), the Natural Science Foundation of Education Bureau of Guizhou Province, China (Grant No QJK 2005105) and Scientific Research Foundation of Young Teacher of Guizhou Normal University, China.
† E-mail: shguangxian@sina.com
‡ Corresponding author. E-mail: xdyang@scu.edu.cn

Vibrational–rotational excitation in atom–molecule collision can be considered as a scattering between a particle and a rotational oscillator in a physical model. It is shown in Fig.1.

Radial equation of vibrational–rotational wavefunction $\phi_{n_rJ_r}(r)$ of diatomic molecule can be expressed as following:

$$\Big[-\frac{\hbar^2}{2\mu_{BC}}\frac{1}{r}\frac{\partial^2}{\partial r^2}r+\frac{J_r(J_r+1)\hbar^2}{2\mu_{BC}r^2}+V_{BC}(r)\Big]\phi_{n_rJ_r}(r) = \varepsilon_{n_rJ_r}\phi_{n_rJ_r}(r). \quad (1)$$

The close coupling equation of radial wavefunction in atom–molecule collisions can be expressed as following:

$$\Big[\frac{\mathrm{d}^2}{\mathrm{d}R^2}-\frac{l_\beta(l_\beta+1)}{R^2}+k^2_{n_\beta J_\beta}\Big]g^J_{n_\beta J_\beta l_\beta,n_aJ_aM_a}(R) = \frac{2\mu_{A,BC}}{\hbar^2}\sum_{n_rJ_rl_r}V^J_{n_\beta J_\beta l_\beta,n_\gamma J_\gamma l_\gamma}(R) \times g^J_{n_\beta J_\beta l_\beta,n_aJ_aM_a}(R). \quad (2)$$

All possible vibrational quantum number n_γ, rotational quantum number l_γ of the atom rotating round molecule, and rotational quantum number J_γ of target molecule itself are summed in right of Eq.(2), and

$$V^J_{n_\beta J_\beta l_\beta n_\gamma J_\gamma {l_\gamma}' J}(R) = \int r^2\mathrm{d}r\phi^*_{n_\beta J_\beta}(r)\phi_{n_\gamma J_\gamma}(r) \times\int \mathrm{d}\hat{r}\mathrm{d}\hat{R}Y^{l_\beta J_\beta}_{JM_\alpha}(\hat{R},\hat{r}) \times[V(R,r,\cos\theta)-V_{BC}(r)] \times Y^{l_\gamma J_\gamma}_{JM_\alpha}(\hat{R},\hat{r}), \quad (3)$$

where $V(R,r,\cos\theta)$ is interactional potential of atom–molecule system, $V_{BC}(r)$ is potential function of diatomic molecule. $V(R,r,\cos\theta)-V_{BC}(r)$ can be expressed as following:

$$V(R,r,\cos\theta)-V_{BC}(r)=\sum_\lambda V^\lambda(R,r)P_\lambda(\cos\theta). \quad (4)$$

Multiplying left side of Eq.(4) by $P_{\lambda'}$ and integrating over $\sin\theta$ we obtain

$$\int P_{\lambda'}(V(R,r,\cos\theta)-V_{BC})\sin\theta\mathrm{d}\theta = \sum_\lambda V^\lambda\int P_\lambda P_{\lambda'}\sin\theta\mathrm{d}\theta=\sum_\lambda V^\lambda\frac{2}{2\lambda'+1}\delta_{\lambda\lambda'},$$

thence the following formula can be obtained

$$V^\lambda(R,r)=\frac{2\lambda+1}{2}\int_0^\pi[V(R,r,\cos\theta)-V_{BC}(r)] \times P_\lambda(\cos\theta)\sin\theta\mathrm{d}\theta. \quad (5)$$

Moreover, in Eq.(2) $V^J_{n_\beta J_\beta l_\beta,n_\gamma J_\gamma l_\gamma}(R)$ can be expressed as

$$V^J_{n_\beta J_\beta l_\beta,n_\gamma J_\gamma l_\gamma}(R)=\sum_\lambda C^{J_\lambda}_{J_\beta l_\beta J_\gamma l_\gamma}V^\lambda_{n_\beta J_\beta n_\gamma J_\gamma}, \quad (6)$$

$$V^\lambda_{n_\beta J_\beta n_\gamma J_\gamma}(R)=\int_0^\infty r^2\mathrm{d}r\phi_{n_\beta J_\beta}(r)V^\lambda(R,r)\phi_{n_\gamma J_\gamma}(r) = \frac{2\lambda+1}{2}\int_0^\pi\int_0^\infty \mathrm{d}r\phi_{n_\beta J_\beta}(r)[V(R,r,\cos\theta) -V_{BC}(r)]P_\lambda(\cos\theta)\phi_{n_\gamma J_\gamma}\sin\theta\mathrm{d}\theta, \quad (7)$$

where $\phi_{n_\beta J_\beta}$ and $\phi_{n_\gamma J_\gamma}$ are vibrational wavefunction.

The interaction potential function of H–H must be calculated to seek the vibrational wavefunction, and then the potential function of He–H_2 will be calculated for calculating the sections of vibrational and rotational excitation in He–H_2 collisions.

The potential function of H–H $\sum_g^+$ can be expressed as

$$V(r)=V_{\mathrm{HF}}(r)-V_{\mathrm{Disp}}(r)-V_{\mathrm{ex}}(r), \quad (8)$$

where $V_{\mathrm{HF}}(r)$ is a calculational result using Hartree–Fork self-consistent-field (SCF) method

$$V_{\mathrm{Disp}}(r)=\sum_{n=3}f_{2n}(r)C_{2n}/r^{2n},$$
$$V_{\mathrm{ex}}(r)=0.821R^{5/2}\mathrm{e}^{-2r}.$$

Substituting the corresponding parts of Eq.(1) into Eq.(8), we can calculate the vibrational wavefunction $\phi_{n_rJ_r}(r)$ of diatomic molecule system.

The interactional potential of He–H_2 collision system has been expressed as

$$V(R,r,\theta)=\sum_{\lambda=0}V_\lambda(R,r)P_\lambda(\cos\theta), \quad (\lambda=0,1,2,\cdots), \quad (9)$$

where $V_\lambda(R,r)$ is radial potential function, $P_\lambda(\cos\theta)$ is Legendre function, and θ is direction angle of atom relative to diatomic molecule. $V(R,r,\theta)$ can be calculated by using trinomial expressions

$$V(R,r,\theta)=V_0(R,r)+V_2(R,r)P_2(\cos\theta) +V_4(R,r)P_4(\cos\theta). \quad (10)$$

Three coefficients of radial potential function related to potential of different directions are obtained.

$$V_0(R,r)=\frac{1}{105}[7V(R,r,0^0)+56V(R,r,45^0)$$

$$+ 42V(R,r,90^0)],$$

$$V_2(R,r) = \frac{2}{105}[25V(R,r,0^0) + 20V(R,r,45^0) - 45V(R,r,90^0)],$$

$$V_4(R,r) = \frac{16}{105}[3V(R,r,0^0) - 6V(R,r,45^0) + 3V(R,r,90^0)]. \quad (11)$$

Every coefficient $V_\lambda(R,r)$ in each term of the Legendre expansion (9) can be represented by a long-range dispersion attractive potential and a short-term SCF repulsive potential[16]

$$V_\lambda(R,r) = A\exp(-bR) - \sum_{2n=0}^{\infty}\Big[1 - \sum_{k=0}^{2n}\frac{(bR)^k}{k!}\exp(-bR)\Big]\frac{C_{2n}}{R^{2n}}. \quad (12)$$

The optical dispersion coefficients C_6^0, C_8^0 and C_{10}^0 of $V_0(R,r)$ at $n = 3,4,5$ can be expressed as following:

$$C_6^0 = P_0 + P_1(r-r_0) + p_2(r-r_0)^2 + P_3(r-r_0)^3,$$
$$C_8^0 = P_0 + P_1(r-r_0) + p_2(r-r_0)^2 + P_3(r-r_0)^3,$$
$$C_{10}^0 = P_0 + P_1(r-r_0) + p_2(r-r_0)^2 + P_3(r-r_0)^3, \quad (13)$$

where $r_0 = 0.449a_0$, values of P_0, P_1, P_2 and P_3 are given in Table 1. Afterwards the C_6^2, C_8^2 and C_{10}^2 of $V_2(R,r)$ at $n = 3,4,5$ are as follows:

$$C_6^2 = \Gamma_6(r)C_6^0, \quad C_8^2 = \Gamma_8(r)C_8^0,$$
$$C_{10}^2 = \Gamma_{10}(r)C_{10}^0, \quad (14)$$

therein

$$\Gamma_{6,8,10}(r) = \frac{ar}{1 + b_1 r + b_2 r^2}, \quad (15)$$

where values of a, b_1 and b_2 are given in Table 2, values of $\Gamma_{6,8,10}$ for different r are given in Table 3.

Table 1. Values of P_0, P_1, P_2 and P_3.

	P_0	P_1	P_2	P_3
$C_6^0(r)$	4.018	2.315	0.0	−0.2622
$C_8^0(r)$	55.500	47.912	11.204	−1.483
$C_{10}^0(r)$	1025.30	1176.182	396.588	−9.897

Table 2. Values of a b_1 and b_2.

	a	b_1	b_2
$\Gamma_6(r)$	0.038686	−0.52500	0.16023
$\Gamma_8(r)$	0.091610	−0.59260	0.13423
$\Gamma_{10}(r)$	0.103700	−0.57550	0.13000

Table 3. Values of $\Gamma_6(r)$, $\Gamma_8(r)$ and $\Gamma_{10}(r)$.

r	$\Gamma_6(r)$	$\Gamma_8(r)$	$\Gamma_{10}(r)$
0.0	0.0	0.0	0.0
0.90	0.05297	0.14329	0.15890
1.28	0.08385	0.25414	0.27865
1.449	0.09736	0.13170	0.34224
1.618	0.10980	0.37757	0.41006
2.00	0.13092	0.52093	0.56206

In the same way, the C_8^4 and C_{10}^4 of $V_4(R,r)$ can be obtained from:

$$C_8^4 = 0.73 + 3.22485(r-r_0) + 4.3766(r-r_0)^2,$$
$$C_{10}^4 = 12.60 + 130.1775(r-r_0) + 1050.3834(r-r_0)^2, \quad (16)$$

with C_6^0, C_8^0, C_{10}^0, C_6^2, C_8^2 and C_{10}^2 given in Table 4.

Table 4. Values of C_6^0, C_8^0, C_{10}^0, C_6^2, C_8^2 and C_{10}^2.

r		C_6^0	C_8^0	C_{10}^0	C_6^2	C_8^2	C_{10}^2
0.0	present	1.461	1.411	1.838	0.0	0.0	0.0
	Ref	1.461[19]	1.411[19]	1.835[19]			
0.9	present	2.79	3.282	5.007	1.478	4.703	7.965
1.28	present	3.628	4.773	8.379	3.04	1.213	2.335
	Ref	3.628[20]	4.773[20]	8.376[20]	3.04[20]	1.213[20]	2.955[20]
1.449	present	4.018	5.550	1.025	3.91	1.741	3.508
	Ref	4.018[20]	5.550[20]	1.025[20]	3.91[20]	1.741[20]	3.509[20]
1.618	present	4.408	6.391	1.235	4.84	2.413	5.064
	Ref	4.018[20]	6.391[20]	1.237[20]	4.84[20]	2.413[20]	4.818[20]
2.0	present	5.250	8.505	1.792	6.873	4.431	1.007

Values of A and b in the Eq.(12) can be calculated by following formula:

$$P = P_0 + P_1(r-r_0) + P_2(r-r_0)^2 + P_3(r-r_0)^3, \quad (17)$$

where $r_0 = 1.449\ a_0$, and P_0, P_1, P_2, and P_3 are given in Table 5. It should be noted that molecular distance r will change when vibration occurs, and $V_\lambda(R,r)$ will change with r and R. Analytical expression V_λ can be obtained by using Eq.(12) when A, b, and C_{2n} change with r, and values of A and b should agree with those of He–He potential at $r = 0$. The values of V_0V_2 and V_4 corresponding to $r = 1.28\ a_0$, $r = 1.449\ a_0$ and $r = 1.618\ a_0$ are given in Table 6.

Table 5. Values of b and A.

		P_0	P_1	P_2	P_3
$V_0(r)$	b	2.0	−0.226006	0.165260	0.098399
	A	14.0	−2.373539	4.900039	2.543710
$V_2(r)$	b	2.122	−0.256310	0.201320	−0.153000
	A	7.9616	5.857905	−0.105038	−0.245550
$V_4(r)$	b	2.30	−0.686580	−0.875320	−1.858060
	A	0.80	0.585963	0.0	−0.016126

Table 6. Values of V_0, V_2 and V_4.

r		1.28	1.449	1.618
$V_0(r)$	b	2.0424	2.0	1.967
	A	14.5288	14.0	13.7511
$V_2(r)$	b	2.1718	2.122	2.0837
	A	6.9698	7.9616	8.9474
$V_4(r)$	b	2.40	2.30	2.15
	A	0.7011	0.80	0.8990

The results of Tables 1–6 accord well with Refs.[19] and [20] which are recognized quite accurate. Precision of section for vibrational excitation in He–H_2 collisions can be ensured because interactional potential of He–H_2 has been calculated accurately.

3. Results and discussion

The energy levels of 00–10, 00–12, 00–14, 00–16 vibrational excitation of H_2, D_2 and T_2 have been calculated, and the results are given in Table 7.

Table 7. Energy levels of vibrational excitation of H_2, D_2 and T_2.

		00–10	00–12	00–14	00–16
E/eV	H_2	0.5162022	0.5579709	0.6539400	0.8005315
	D_2	0.3711843	0.3925993	0.4421835	0.519015
	T_2	0.30531046	0.3197416	0.3532416	0.405395

According to Table 7, the vibrational and rotational energy gaps of H_2 are the largest, followed by those of D_2 the larger and those of T_2 the smallest.

The partial cross sections for vibrational excitation in He–H_2(D_2, T_2) collisions are studied by using a series of incident energy $E = 0.55$, 0.65 and 0.75 eV respectively. The results are given in Figs.2–12.

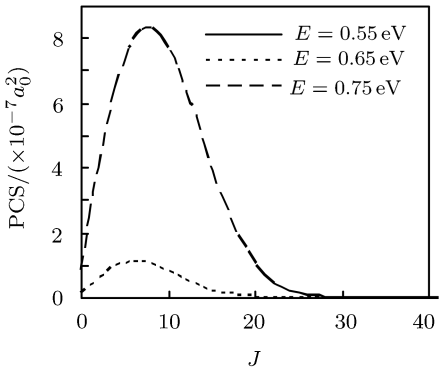


Fig.2. Partial cross section 00–10 for vibrational excitation in He–H_2 collisions.

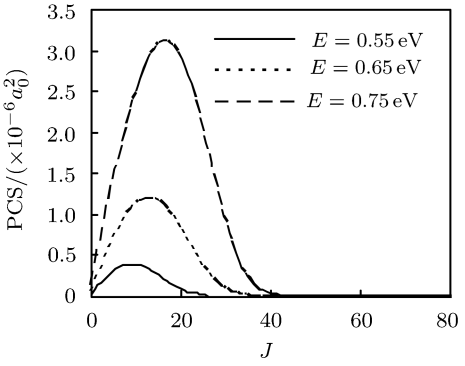


Fig.3. Partial cross section 00–10 for vibrational excitation in He–D_2 collisions.

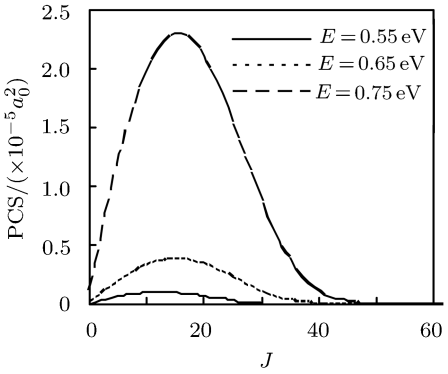


Fig.4. Partial cross section 00–10 for vibrational excitation in He–T_2 collisions.

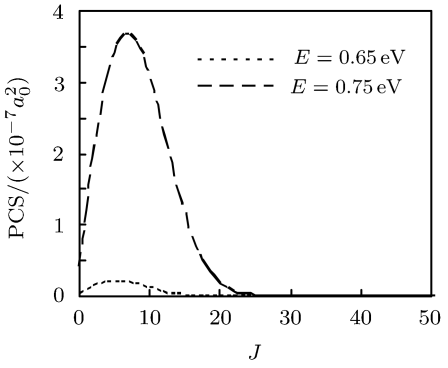


Fig.5. Partial cross section 00–12 for vibrational excitation in He–H_2 collisions.

According to Figs.2–12, the following conclusions can be drawn:

When incident energy and the reduced mass are different, for first vibrational excitation in He–H_2(D_2, T_2) collision, the curvilinear figures of the partial cross sections changing with J are similar, which is following: the sections reach a maximum at first, and then tend toward zero rapidly, but the peak value and converging speed are different greatly.

(1) For same incident atom, as the incident energy is determined, the peak value of partial section went up with the increases of mass of isotope molecule. That is brought by difference of vibrational and rotational energy gaps mostly. As the energy gaps of T_2 are the smallest among H_2, D_2 and T_2, the probability of He–T_2 system excited to energy levels of $vj\rangle = 10$ becomes the largest, then the peak values for section of rotational and vibrational excitation are the largest, followed by those of He–D_2 system larger and of He–H_2 system smallest. Owing to the largest energy gaps of He–H_2 system, excitations to energy levels of $vj\rangle = 12$ when the incident energy $E = 0.55$ eV, to energy levels of $vj\rangle = 14$ when $E = 0.65$ eV and to energy level of $vj\rangle = 16$ when $E = 0.75$ eV are impossible.

(2) The peak value of partial section of vibrational excitation, the position of scattering maximum and the converging speed will change with the change of incident energy of atom and the reduced mass of system. The values are given in Tables 8 and 9 respectively.

Table 8. Max. value of partial section of vibrational excitation and quantum number.

E/eV		0.55		0.65		0.75	
		Max.value/a_0^2	J	Max.value/a_0^2	J	Max.value/a_0^2	J
H_2	00–10	1.469×10^{-9}	4	1.094×10^{-7}	6	8.293×10^{-7}	8
	00–12			2.073×10^{-8}	5	3.666×10^{-7}	7
	00–14					8.558×10^{-9}	6
	00–16						
D_2	00–10	3.982×10^{-7}	9	1.202×10^{-6}	13	3.110×10^{-6}	16
	00–12	2.128×10^{-7}	7	2.367×10^{-6}	9	7.765×10^{-6}	12
	00–14	1.786×10^{-8}	7	5.590×10^{-7}	9	4.056×10^{-6}	10
	00–16	4.974×10^{-11}	8	1.539×10^{-8}	9	2.977×10^{-7}	11
T_2	00–10	1.035×10^{-6}	12	3.780×10^{-6}	15	2.289×10^{-5}	16
	00–12	6.789×10^{-7}	9	3.986×10^{-6}	11	3.050×10^{-5}	12
	00–14	1.775×10^{-7}	9	1.240×10^{-6}	10	9.524×10^{-6}	11
	00–16	1.473×10^{-8}	11	2.175×10^{-7}	13	1.456×10^{-6}	14

Table 9. Converging quantum number of partial section of vibrational excitation (J).

E/eV	H_2				D_2				T_2			
	00–10	00–12	00–14	00–16	00–10	00–12	00–14	00–16	00–10	00–12	00–14	00–16
0.55	15				27	21	19	18	32	25	30	25
0.65	21	16			36	32	30	25	41	38	40	35
0.75	29	26	25		45	43	40	36	49	50	48	46

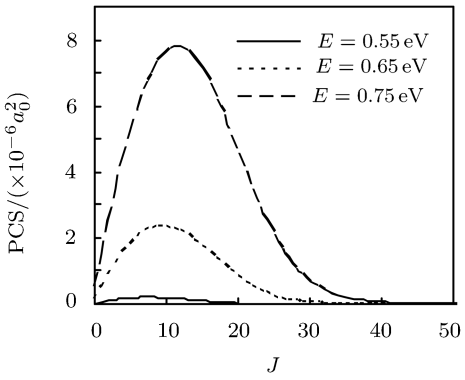


Fig.6. Partial cross section 00–12 for vibrational excitation in He–D_2 collisions.

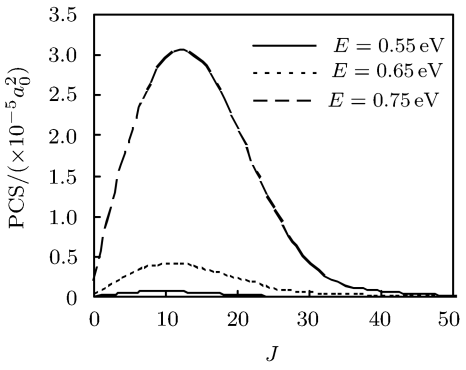


Fig.7. Partial cross section 00–12 for vibrational excitation in He–T_2 collisions.

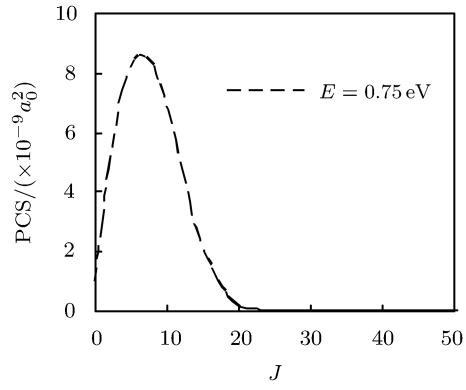


Fig.8. Partial cross section 00–14 for vibrational excitation in He–H_2 collisions.

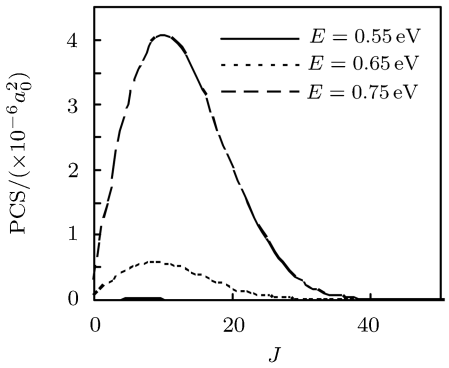


Fig.9. Partial cross section 00–14 for vibrational excitation in He–D_2 collisions.

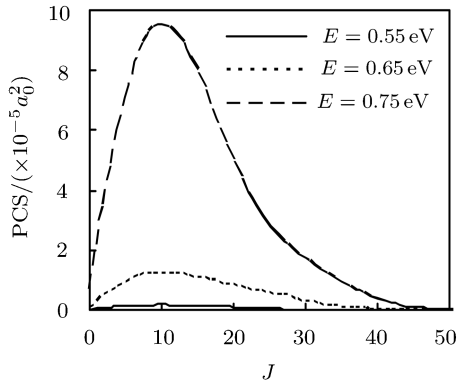


Fig.10. Partial cross section 00–14 for vibrational excitation in He–T_2 collisions.

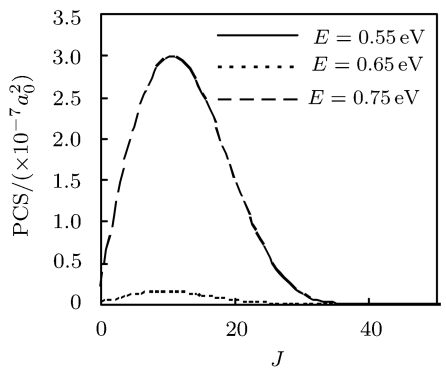


Fig.11. Partial cross section 00–16 for vibrational excitation in He–D_2 collisions.

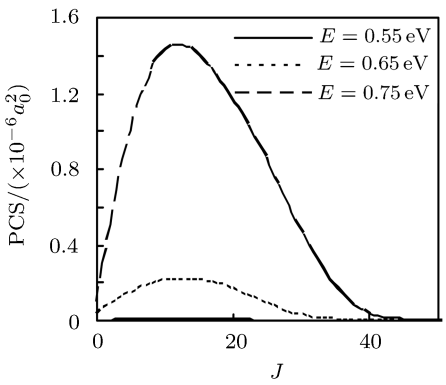


Fig.12. Partial cross section 00–16 for vibrational excitation in He–T_2 collisions.

According to Table 8, as the incident energy is determined, it can be seen easily that the change rules of maximum value of partial section of vibrational excitation are as following:

$$\sigma_{00-10}(H_2) < \sigma_{00-10}(D_2) < \sigma_{00-10}(T_2),$$
$$\sigma_{00-12}(H_2) < \sigma_{00-12}(D_2) < \sigma_{00-12}(T_2),$$
$$\sigma_{00-14}(H_2) < \sigma_{00-14}(D_2) < \sigma_{00-14}(T_2),$$
$$\sigma_{00-16}(H_2) < \sigma_{00-16}(D_2) < \sigma_{00-16}(T_2).$$

As the reduced mass of system is determined, the change rules of maximum value of partial section of vibrational excitation are as following:

$$\sigma_{E=0.55\,eV}(H_2) < \sigma_{E=0.65\,eV}(H_2) < \sigma_{E=0.75\,eV}(H_2),$$
$$\sigma_{E=0.55\,eV}(D_2) < \sigma_{E=0.65\,eV}(D_2) < \sigma_{E=0.75\,eV}(D_2),$$
$$\sigma_{E=0.55\,eV}(T_2) < \sigma_{E=0.65\,eV}(T_2) < \sigma_{E=0.75\,eV}(T_2).$$

According to Table 9, as the incident energy is determined, it can be seen easily that the change rules of converging quantum number J of partial section of vibrational excitation are as following:

$$J_{00-10}(H_2) < J_{00-10}(D_2) < J_{00-10}(T_2),$$
$$J_{00-12}(H_2) < J_{00-12}(D_2) < J_{00-12}(T_2),$$
$$J_{00-14}(H_2) < J_{00-14}(D_2) < J_{00-14}(T_2),$$
$$J_{00-16}(H_2) < J_{00-16}(D_2) < J_{00-16}(T_2).$$

As the reduced mass of system is determined, the change rules of converging quantum number J of partial section of vibrational excitation are as following:

$$J_{E=0.55\,eV}(H_2) < J_{E=0.65\,eV}(H_2) < J_{E=0.75\,eV}(H_2),$$
$$J_{E=0.55\,eV}(D_2) < J_{E=0.65\,eV}(D_2) < J_{E=0.75\,eV}(D_2),$$
$$J_{E=0.55\,eV}(T_2) < J_{E=0.65\,eV}(T_2) < J_{E=0.75\,eV}(T_2).$$

4. Conclusions

Based on above discussion for He–H_2(D_2, T_2) collisions system, we can summarize as follows:

(1) As the relative incident energy of atom is determined, the positions of peak value of partial section of 00–10, 00–12, 00–14, 00–16 vibrational excitation shift towards large values of J with the increasing reduced mass of system, respectively. As the reduced mass of system is determined, the positions of peak value of partial section of vibrational excitation shift similarly towards large values of J with the increasing incident energy, and the maximum values of section increase gradually.

(2) As the incident energy is determined, the converging speed slows down with the increasing reduced mass. And as the reduced mass of system is determined, the converging speed slows down with the increasing incident energy, similarly.

References

[1] Yang X D 1990 *Sci. Chin.* A **8** 833
[2] Yu C R, Huang S Z, Feng E Y, Wang R K, Cheng X L and Yang X D 2006 *Acta Phys. Sin.* **55** 2215 (in Chinese)
[3] Yu C R, Feng E Y, Wang R K and Yang X D 2006 *Chin. Phys.* **15** 2571
[4] Yang C L and Zhu Z H 1999 *Acta Phys. Sin.* **48** 1852 (in Chinese)
[5] Jiang G, Xie H P, Tan M L and Zhu Z H 2000 *Acta Phys. Sin.* **49** 665 (in Chinese)
[6] Wang R K, Linghu R F and Yang X D 2007 *Acta Phys. Sin.* **56** 2067 (in Chinese)
[7] Yu C R, Wang R K, Chen X L and Yang X D 2007 *Acta Phys. Sin.* **56** 2577 (in Chinese)
[8] Yu C R and Yang X D 2007 *Acta Phys. Sin.* **56** 4441 (in Chinese)
[9] Yang X D, Zhang J Y and Jing F Q 1998 *Chin. Phys. Lett.* **15** 19
[10] Manson J T 1999 *Chin. Phys.* **8** 313
[11] Yang X D, Zhou X L, Zhang J Y, Sun G H and Zhu J 2002 *Chin. Phys.* **11** 1013
[12] Gurtiss C F 1970 *J. Chem. Phys.* **52** 1078
[13] Gordon M D and Secrest D 1970 *J. Chem. Phys.* **52** 120
[14] Tang K T and Toennies J P 1981 *J. Chem. Phys.* **74** 114
[15] Feng Y B, Zhang J Y and Jiang D Q 2000 *J. At. Mo1. Phys.* **17** 477 (in Chinese)
[16] Jiang D Q and Yang X D 2001 *J. Sichuan University* (Natural Science Edition) **24** (6) 580 (in Chinese)
[17] Jiang D Q, Wang X Q and Yang X D 2002 *J. At. Mo1. Phys.* **19** 75 (in Chinese)
[18] Jiang D Q, Li X and Wei Q 2003 *J. Sichuan University* (Natural Science Edition) **26** (5) 486 (in Chinese)
[19] Meyer W 1980 *J. Chem. Phys.* **73** 1880
[20] Tang K T and Toennies J P 1986 *Z. Phys.* D **1** 91