Vol 17 No 6, June 2008
1674-1056/2008/17(06)/2090-07

Chinese Physics B

© 2008 Chin. Phys. Soc.
and IOP Publishing Ltd

Elastic scattering of two H(^2S_g) and N(^4S_u) atoms at low temperatures and accurate spectroscopic parameters of NH ($X^3\Sigma^-$) radical*

Shi De-Heng(施德恒)[a)b)†], Zhang Jin-Ping(张金平)[a)], Sun Jin-Feng(孙金锋)[b)], Zhu Zun-Lüe(朱遵略)[b)], Liu Yu-Fang(刘玉芳)[b)], and Yang Xiang-Dong(杨向东)[c)]

[a)] *College of Physics & Electronic Engineering, Xinyang Normal University, Xinyang* 464000, *China*
[b)] *College of Physics & Information Engineering, Henan Normal University,Xinxiang* 453007, *China*
[c)] *Institute of Atomic & Molecular Physics, Sichuan University, Chengdu* 610065, *China*

(Received 3 September 2007; revised manuscript received 14 October 2007)

This paper reports that the interaction potential for the $X^3\Sigma^-$ state of NH radical is constructed at the CCSD(T)/cc-PV6Z level of theory. Using this potential, this paper calculates the spectroscopic parameters (D_e, R_e, ω_e, $\omega_e\chi_e$, α_e and B_e) and their values are of 3.578 eV, 0.10368 nm, 3286.833 cm^{-1}, 78.433 cm^{-1}, 0.6469 cm^{-1} and 16.6735 cm^{-1}, respectively, which are in excellent agreement with the experiments. Then the total of 14 vibrational states has been found when J=0 by solving the radial Schrödinger equation of nuclear motion. For each vibrational state, the vibrational manifolds are reported for the first time. And last, the total cross sections, s-wave, p-wave and d-wave cross sections are computed for the elastic collisions between two ground-state atoms (hydrogen and nitrogen) at low temperatures. It finds that the total elastic cross sections are dominated by s-wave scattering when the collision energy is below 10^{-6}a.u. The pronounced shape resonance is found at energy of 6.1×10^{-6}a.u. Calculations have shown that the shape resonance comes from the p-wave contributions.

Keywords: atomic collision, total elastic cross section, shape resonance, partial-wave cross section, spectroscopic parameter

PACC: 3440, 3400, 3430

1. Introduction

NH radical is of fundamental importance. It plays a significant role in many chemical processes, including combustion. It has also been identified in stellar atmospheres and in comets through transitions in its electronic, vibration–rotation and high-N rotational spectra.[1,2] Recently, the N=2–1 transition of this radical has been detected in the direction of Sagittarius $B2$ as part of the Infrared Space Observatory (ISO) program.[3] A knowledge of the abundance of NH in dark clouds is very important for the study of nitrogen chemistry because it is likely to be an intermediate in the formation of NH_3 by successive hydrogenation reactions.[4,5]

In theories, the *ab initio* calculations on the $X^3\Sigma^-$ state of this radical have been carried out extensively. But to the best of our knowledge, only several investigations[6−9] can give satisfactory spectroscopic parameters, and the extracted spectroscopic properties from these investigations are all incomplete. For example, we have not found any results about its vibrational levels, classical turning points and inertial rotation and centrifugal distortion constants, which are very useful in the theoretical rovibrational transition calculations. In experiments, it is noteworthy that the value of its dissociation energy varies significantly.[10−12] And up to now, the accurate dissociation energy has not been determined experimentally. Meanwhile, because the elastic collision properties, such as the total and the partial-wave cross sections, are very sensitive to the interaction potential over an extended range of internuclear distances, no investigations can be found about the elastic scattering between two ground-state H and N atoms in the cold regime due to the lack of accurate analytic

*Project supported by the National Natural Science Foundation of China (Grant No 10574039), Science and Technology Innovation Talents in Universities of Henan Province in China (Grant No 2008HASTIT008) and the Natural Science Foundation of Education Bureau of Henan Province, China (Grant No 2007140015).
†E-mail: dehengshi@yahoo.com.cn

potential energy function (APEF).

One of the purposes of the present work is to construct the reliable APEF of this NH ($X^3\Sigma^-$) radical using the coupled-cluster singles-doubles-approximate-triples [CCSD(T)] theory[13] in combination with the correlation-consistent sextuple basis set (cc-PV6Z).[14−16] In Section 2, we briefly describe the low-energy elastic scattering theory. In Section 3, we calculate the accurate APEF, spectroscopic parameters and vibrational manifolds. In Section 4, we compute the total, s-wave, p-wave and d-wave cross sections for the elastic scattering between two ground-state atoms (nitrogen and hydrogen) at low temperatures. And in Section 5, concluding remarks are made. Atomic units are employed throughout this paper otherwise specified.

2. Low-energy elastic scattering theory

The theory of scattering by a potential $V(r)$, where r is the internuclear distance of two atoms, can be described by the following radial Schrödinger equation,[17]

$$\frac{\mathrm{d}^2u_l}{\mathrm{d}r^2}+\left[k^2-\frac{2\mu V(r)}{\hbar^2}-\frac{l(l+1)}{r^2}\right]u_l(r)=0, \qquad (1)$$

where μ is the reduced mass of the colliding system and k is the wave number given in terms of the energy E of relative motion by $k^2=2\mu E/\hbar^2$, $V(r)$ is the diatomic interaction potential. The solution must be regular and behave asymptotically as the following formula when $r\to\infty$:

$$u_l(r)\sim A_l[j_l(kr)+\tan\delta_l n_l(kr)]. \qquad (2)$$

Where j_l and n_l are, respectively, the spherical Bessel and Neumann functions. A_l is an arbitrary amplitude, and δ_l is the scattering phase shift of the lth partial wave. Alternatively, we can write

$$u_l(r)\sim A_l\sin\left(kr-\frac{1}{2}l\pi+\delta_l\right). \qquad (3)$$

If A_l is chosen to equal unity, the solution $u_l(r)$ satisfies the following integral equation:[18]

$$\tan\delta_l=\frac{-2\mu}{\hbar^2k}\int_0^\infty j_l(kr)V(r)u_l(r)\mathrm{d}r. \qquad (4)$$

When l equals 0, 1, 2, $\cdots$, the scattering waves are usually called s partial wave, p partial wave, d partial wave, $\cdots$, respectively. The elastic cross section of lth partial wave, $\sigma_l(E)$, can be calculated by[19]

$$\sigma_l(E)=\frac{4\pi}{k^2}\cdot(2l+1)\sin^2\delta_l. \qquad (5)$$

Then, the total elastic cross section, $\sigma_T(E)$, can be defined as

$$\sigma_T(E)=\sum_{l=0}^{\infty}\sigma_l(E)=\frac{4\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)\sin^2\delta_l. \qquad (6)$$

With the accurate diatomic interaction potential derived from Gaussian 03 program package,[20] the $u_l(r)$ can be obtained by solving the radial Schrödinger equation (1). Once the $u_l(r)$ is attained, various cross sections for the elastic collisions of two ground-state hydrogen and nitrogen atoms in the cold regime can be easily calculated according to Eqs.(5) and (6).

3. Interaction potential

The calculations about the equilibrium structure and the frequency of this NH ($X^3\Sigma^-$) radical are performed in Gaussian 03 program package[20] at a series of the correlation-consistent basis sets of Dunning and co-workers.[14−16] The D_e, R_e and ω_e calculation results are all tabulated in Table 1. By careful comparison between the calculated values and the experiments,[10−12,21−23] we are certain that the correlation-consistent sextuple basis set, cc-PV6Z, is an excellent one.

Table 1. The equilibrium parameters for NH ($X^3\Sigma^-$) radical at the CCSD (T) level of theory and the different correlation-consistent basis sets.

basis sets	D_e/eV	R_e/nm	ω_e/cm^{-1}	basis sets	D_e/eV	R_e/nm	ω_e/cm^{-1}
cc-PVDZ	3.097	0.10560	3196.638	aug-cc-PVDZ	3.250	0.10518	3212.191
cc-PVTZ	3.434	0.10392	3267.614	aug-cc-PVTZ	3.494	0.10395	3264.919
cc-PVQZ	3.533	0.10372	3282.320	aug-cc-PVQZ	3.556	0.10375	3281.994
cc-PV5Z	3.566	0.10369	3285.848	aug-cc-PV5Z	3.574	0.10370	3285.181
cc-PV6Z	3.578	0.10368	3286.833				

The potential energy curve (PEC) of the ground-state NH radical is calculated at the cc-PV6Z basis set over the internuclear distance range from 0.07 to 2.62 nm. And the following common M-S function[24] is used to describe its APEF,

$$V(\rho) = -D_{\rm e}\left(1+\sum_{i=1}^{n} a_i\rho^i\right)\exp(-a_1\rho). \qquad (7)$$

Where, $\rho = R - R_{\rm e}$, R is the internuclear distance of a diatomic molecule. $R_{\rm e}$ is its equilibrium internuclear separation and is regarded as a fixed parameter in the fitting process. The dissociation energy $D_{\rm e}$ and the parameters a_i are determined by fitting.

Fitting equation (7) by the least-squares method, we obtain the parameters a_i and $D_{\rm e}$. In order to obtain a satisfactory result, we try it from n=3 to n=8, and find the best results at n=6. The fitting results are tabulated in Table 2 together with the $R_{\rm e}$ value for integrality.

Table 2. Parameters of M–S APEF for NH ($X^3\Sigma^-$) at the CCSD(T)/cc-PV6Z level of theory.

$D_{\rm e}$/eV	$R_{\rm e}$/nm	a_1/nm^{-1}	a_2/nm^{-2}	a_3/nm^{-3}	a_4/nm^{-4}	a_5/nm^{-5}	a_6/nm^{-6}	RMSE/eV
3.578	1.0368	45.2219	516.1831	3817.561	–20719.17	–589910.22	3116541.5	0.00218

To appreciate the fitting quality of this APEF, we calculate the $\Delta E_{\rm RMSE}$ in the fitting process,

$$\Delta E_{\rm EMSE} = \sqrt{\frac{1}{N}\left[\sum_{i=1}^{N}(V_{\rm APEF} - V_{ab\ initio})^2\right]}. \qquad (8)$$

Where $V_{\rm APEF}$ and $V_{ab\ initio}$ are energies attained by the fitting and by the *ab initio* calculations, respectively. N is the number of fitting points (here N=87). The present $\Delta E_{\rm RMSE}$ is of only 0.00218 eV (about 0.0504 Kcal/mol). Obviously, our fitting accuracy is greatly superior to the chemical accuracy (1.0 Kcal/mol).[25] It shows that the M-S function is very suitable for reproducing the PEC of this NH ($X^3\Sigma^-$) radical, and the fitting process is of high quality. Therefore, the present APEF collected in Table 2 is credible.

In order to test the APEF constructed above, now we calculate the spectroscopic parameters and the vibrational manifolds, and compare them with the experiments wherever available. Based on the APEF tabulated in Table 2, the force parameters, quadratic f_2, cubic f_3 and quartic f_4, are calculated, and then the spectroscopic parameters, $\omega_{\rm e}\chi_{\rm e}$, $\alpha_{\rm e}$ and $B_{\rm e}$, are determined as per the method given in Refs.[26–28]. These values together with the available experimental[10−12,21−23] and other valuable theoretical[6−9] results are collected in Table 3.

In Table 3, one can find that the $R_{\rm e}$, $\omega_{\rm e}$, $B_{\rm e}$, $\omega_{\rm e}\chi_{\rm e}$ and $\alpha_{\rm e}$ values are in accord with the measurements[10] within 0.056%, 0.139%, 0.154%, 0.106% and 0.323% respectively, and are also in agreement with the experiments[21] within 0.039%, 0.117%, 0.039%, 0.555% and 0.108% respectively. According to these, we conclude that the $D_{\rm e}$ value obtained at cc-PV6Z is accurate and the APEF fitted is credible.

Table 3. Spectroscopic parameter comparison with the measurements and other theories for NH ($X^3\Sigma^-$) at the CCSD(T)/cc-PV6Z level of theory.

Source	$D_{\rm e}$/eV	$R_{\rm e}$/nm	$\omega_{\rm e}$/cm^{-1}	$B_{\rm e}$/cm^{-1}	$\alpha_{\rm e}$/cm^{-1}	$\omega_{\rm e}\chi_{\rm e}$/cm^{-1}
This work	3.578	0.10368	3286.833	16.6735	0.6469	78.433
Exp.[10]	≤3.671	0.10362	3282.27	16.6993	0.6490	78.35
Exp.[11]	D_0=3.40±0.16	—	—	—	—	—
Exp.[12]	3.386≤ $D_{\rm e}$ ≤3.667	—	—	—	—	—
Exp.[21]	—	0.10372	3283	16.6670	0.6476	78
Exp.[22]	—	0.10376	3282.583	—	—	78.915
Exp.[23]	—	0.1037	3282.1	16.67	0.648	78.3
Theory[6]	3.580	0.1039	3269.3	16.60	0.648	78.8
Theory[7]	3.516	0.10371	3279.4	16.671	0.6522	78.7
Theory[8]	3.600	0.10363	3282.64	—	—	79.097
Theory[9]	3.591	0.1037	3284	16.665	0.659	81

The earlier investigations about NH ($X^3\Sigma^-$) radical were performed by Meyer *et al*[6] Meyer *et al* calculated the D_e, R_e and ω_e values using the coupled electron pair approach with the Gaussian type orbitals, which comprised 4s, 4p, 2d and 1f functions for N and 4s, 2p, 1d for H atom. As we see, their ω_e value from the measurements[10] are too small by 12.97 cm^{-1}. Peterson *et al*[7] used a number of methods and basis sets for a series of benchmark calculations. And the best results were obtained at the CASSCF+1+2/cc-PV5Z level of theory. Lately, Martin[8] used the CCSD(T) method with the AUG-cc-PV5Zuc basis set, and Hirata *et al*[9] combined the DK3-CCSD, DK3-CCSDT and DK3-CCSDTQ theories with the cc-PVTZ, cc-PVQZ and cc-PV5Z basis sets to carry out the sophisticated calculations so as to attain the accurate R_e, D_e and ω_e. From Table 3, we find that the accuracy of these calculations[7−9] is equivalent to ours. However, we should notice that these calculations did not give the expression of the APEF, which is very useful in the elastic collision investigations, and did not make the vibrational manifold calculations, either. Therefore, the present investigations are more complete when compared with previous theories.

In the adiabatic approximation, the vibrational levels of a given electronic state of a diatomic molecule can be obtained by solving the following radial Schrödinger equation of nuclear motion,

$$\left[-\frac{\hbar^2}{2\mu}\frac{\mathrm{d}^2}{\mathrm{d}r^2}+\frac{\hbar^2}{2\mu r^2}J(J+1)+V(r)\right]\Psi_{\nu,J}(r) = E_{\nu,J}\,\Psi_{\nu,J}(r). \quad (9)$$

Here $V(r)$ is the adiabatic rotationless APEF tabulated in Table 2, ν and J are the vibrational and rotational quantum numbers, respectively, μ is the reduced mass of this NH radical. The rotational sublevel of a given vibrational level is represented by the following power series:[29]

$$\begin{aligned}E_{\nu,J} =& G(\nu)+B_\nu[J(J+1)]-D_\nu[J(J+1)]^2\\ &+H_\nu[J(J+1)]^3+L_\nu[J(J+1)]^4\\ &+M_\nu[J(J+1)]^5+N_\nu[J(J+1)]^6\\ &+O_\nu[J(J+1)]^7. \end{aligned}\quad (10)$$

By solving Eq.(9) numerically, we have obtained a total of 14 vibrational states for NH ($X^3\Sigma^-$) with zero angular momentum. For each vibrational state, 1 vibrational level, $G(\nu)$, 1 inertial rotation constant, B_ν, and 6 centrifugal distortion constants, D_ν, H_ν, L_ν, M_ν, N_ν and O_ν, are obtained. They are collected in Tables 3 and 4, respectively.

Unfortunately, we have not found any measurements about the vibrational levels, classical turning points, inertial rotation and centrifugal distortion constants for this NH ($X^3\Sigma^-$) radical. Thus we cannot make any direct comparison. But according to the high-quality fitting process of the APEF and the good agreement between the present spectroscopic parameters and the measurements, [10−12,21−23] we have reasons to believe that the results collected in Tables 3 and 4 are reliable.

Table 4. The vibrational levels, classical turning points and inertial rotation constants for the vibrational states of NH ($X^3\Sigma^-$) at the CCSD(T)/cc-PV6Z level of theory.

ν	$G(\nu)$/cm^{-1}	R_{min}/nm	R_{max}/nm	B_ν/cm^{-1}	ν	$G(\nu)$/cm^{-1}	R_{min}/nm	R_{max}/nm	B_ν/cm^{-1}
0	1607.032	0.094291	0.11555	16.346635	7	20366.699	0.077054	0.17319	11.834296
1	4710.500	0.088704	0.12615	15.704974	8	22402.851	0.076112	0.18202	11.063115
2	7681.149	0.085375	0.13461	15.083671	9	24235.923	0.075317	0.19194	10.203858
3	10516.290	0.082947	0.14236	14.468806	10	25840.187	0.074656	0.20361	9.2125054
4	13210.780	0.081036	0.14985	13.848301	11	27178.308	0.074128	0.21845	8.0031690
5	15757.342	0.079472	0.15734	13.210721	12	28188.267	0.073742	0.24043	6.3542717
6	18146.581	0.078162	0.16505	12.544064	13	28739.361	0.073535	0.30177	3.4463196

Table 5. The centrifugal distortion constants for the vibrational states of NH ($X^3\Sigma^-$) with zero angular momentum at the CCSD(T)/cc-PV6Z level of theory.

ν	$-D_\nu(\times10^{-3})$/cm^{-1}	H_ν $(\times10^{-7})$/cm^{-1}	$L_\nu(\times10^{-11})$/cm^{-1}	$M_\nu(\times10^{-15})$/cm^{-1}	$N_\nu(\times10^{-18})$/cm^{-1}	$O_\nu(\times10^{-21})$/cm^{-1}
0	–1.7317969	1.2846276	–0.8263930	0.8088030	–0.5754976	0.08859022
1	–1.6659806	1.2277890	–1.4390066	1.4204445	–0.5016368	0.08097689
2	–1.6218545	1.1363109	–1.8877028	1.8771611	–0.6646046	0.07340355
3	–1.5978920	1.0201792	–2.2897812	1.9314345	–0.9825752	0.05008582

Table 5. (*Continued*)

ν	$-D_\nu(\times10^{-3})/\mathrm{cm}^{-1}$	H_ν $(\times10^{-7})/\mathrm{cm}^{-1}$	$L_\nu(\times10^{-11})/\mathrm{cm}^{-1}$	$M_\nu(\times10^{-15})/\mathrm{cm}^{-1}$	$N_\nu(\times10^{-18})/\mathrm{cm}^{-1}$	$O_\nu(\times10^{-21})/\mathrm{cm}^{-1}$
4	–1.5935647	0.8752964	–2.7530113	1.3575978	–1.5199686	–0.04930495
5	–1.6099059	0.6853063	–3.4100506	–0.3400751	–2.5483739	–0.37895343
6	–1.6502241	0.4171389	–4.4863563	–4.4122981	–4.8535274	–1.4194429
7	–1.7214728	0.0063941	–6.4595722	–14.243950	–10.896786	–4.9414604
8	–1.8372641	–0.6819404	–10.519883	–40.221567	–29.762286	–18.881160
9	–2.0252423	–1.9695143	–20.199271	–121.03629	–103.91571	–90.089906
10	–2.3482242	–4.7842847	–48.894343	–451.06984	–518.29074	–642.15369
11	–2.9825600	–12.784771	–172.99096	–2662.1149	–4859.5006	–9807.9469
12	–4.6811560	–52.588606	–1388.1988	–46483.793	–181908.26	–786132.27
13	–11.415473	–211.41380	4957.1590	1019481.4	3186539.3	–70535637

4. Total and partial-wave elastic cross sections

Employing the potential tabulated in Table 2, we can numerically solve Eq.(1) by the Numerov method. The partial-wave phase shift δ_l of the elastic collisions between two ground-state hydrogen and nitrogen atoms for the ground state $X^3\Sigma^-$ of this NH radical is calculated according to the formula (4). The elastic partial-wave cross sections and the total elastic cross sections are calculated by using Eqs.(5) and (6). The collision energy dependence of the total elastic cross sections calculated at low and ultralow temperatures is shown in Fig.1. The collision energy dependences of the s-wave, p-wave and d-wave elastic cross sections are depicted in Figs.2–4, respectively.

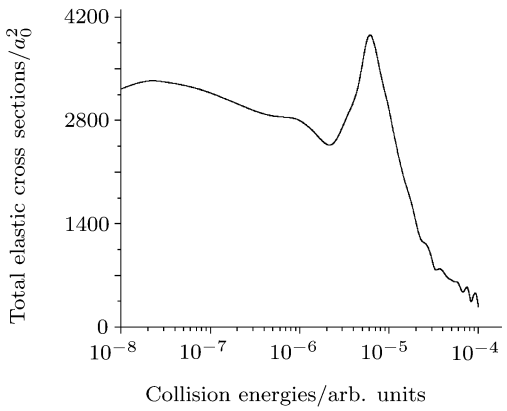


Fig.1. Total cross sections for elastic scattering between two ground-state atoms, N and H, in the ground state of NH radical.

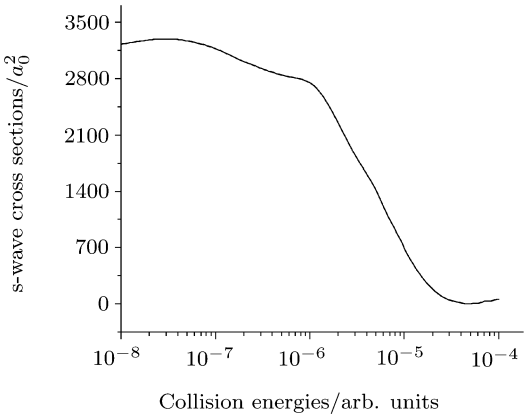


Fig.2. s-wave cross sections for elastic scattering between the two ground-state atoms, N and H, in the ground-state NH radical.

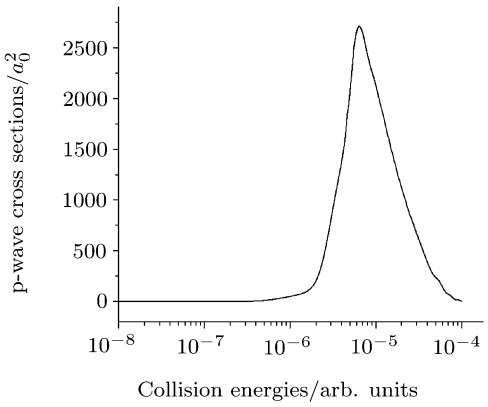


Fig.3. p-wave cross sections for elastic scattering between two ground-state atoms, N and H, in the ground-state NH radical.

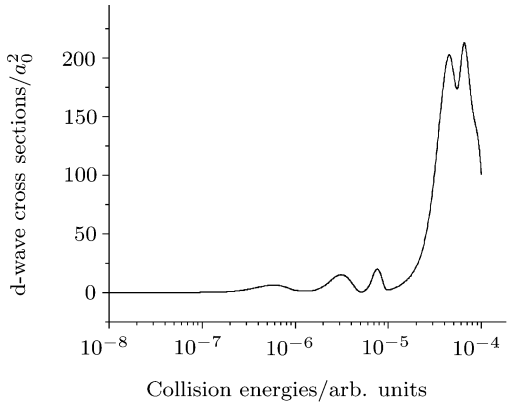


Fig.4. d-wave cross sections for elastic scattering between two ground-state atoms, N and H, in the ground-state NH radical.

As shown in Fig.1, the total cross sections of elastic collisions between two ground-state atoms, hydrogen and nitrogen, are very large and are almost constant at ultralow temperatures. From Figs.2–4, we can see that the s-wave cross sections are significant when the energy is below 10^{-6} a.u.. Thus the total elastic cross sections are dominated by s-wave scattering at this energy range. With the increase of energy, the s-wave cross section tends to decrease, but the decrease is obviously overcome by the higher partial-wave contributions, which initially increase with impact energy from zero before passing through maximum. As shown in Figs.1 and 4, small oscillations occur by the addition of d partial wave around the energies of 4.0–9.0$\times10^{-5}$ a.u..

A sharp structure can be found in Fig.1. From Figs.2–4, one can see that this sharp structure results from the shape resonance. Obviously, the most prominent of this shape resonance comes from the p-wave contributions. For the low-energy atomic collisions, because the collision energy of ultracold atoms is lower than the centrifugal barrier, the shape resonance that is associated with quasi-bound state trapped by the centrifugal barrier is important. Accurate calculations show that the pronounced shape resonance occurs at energy of 6.1×10^{-6} a.u. It is consistent with the resonant position of p partial wave.

We have investigated the elastic collisions of two Li atoms at low and ultralow energy ranges using the present theoretical method.[17] The attained results are in excellent agreement with the experiments. Meanwhile, the above analyses have shown that the interaction potential constructed in this paper is reliable and accurate. Therefore, though no experimental and theoretical results can be found about the elastic collisions between two N and H atoms at low and ultralow energy ranges, we believe that various elastic cross sections calculated at low temperatures are reliable and accurate. These results are expected to be tested by experiments and other theories in the future.

5. Conclusions

We have constructed the accurate potential at the CCSD(T)/cc-PV6Z level of theory. Using this potential, we have calculated the spectroscopic parameters and the vibrational manifolds. Excellent agreement is found when comparing them with the experiments wherever available. The elastic scattering properties, such as the total elastic cross sections, s-wave, p-wave and d-wave cross sections are investigated for the first time by using the present potential. It has been found that the total elastic cross sections are almost constant and are dominated by s-wave scattering when the collision energy is below 10^{-6} a.u.. The pronounced shape resonance in the total elastic cross sections, which may be detected experimentally in the future, is found at energy of 6.1×10^{-6} a.u.. Calculations have pointed out that the shape resonance comes from the p-wave contributions.

Acknowledgments

We heartily thank Professor Zhu Zheng-He, of Sichuan University, for helpful discussion about the arithmetic of vibrational manifolds during the planning stages of this work.

References

[1] Lambert D L, Brown J A, Hinkle K H and Johnson H R 1984 *Astrophys. J.* **284** 223
[2] Meyer D M and Roth K C 1991 *Astrophys. J. Lett.* **376** L49
[3] Cernicharo J, Goioechea J R and Caux E 2000 *Astrophys. J. Lett.* **534** L199
[4] Mann A P C and Williams D A 1984 *Month Not. R. Astron. Soc.* **209** 33
[5] Wagenblast R, Williams D A, Millar T J and Nejad L A M 1993 *Month Not. R. Astron. Soc.* **260** 420
[6] Mayer W and Rosmus P 1975 *J. Chem. Phys.* **63** 2356
[7] Peterson K A, Kendall R A and Dunning T H 1993 *J. Chem. Phys.* **99** 1930
[8] Martin J M L 1998 *Chem. Phys. Lett.* **292** 411

[9] Hirata S, Yanai T, de Jong W A, Nakajima T and Hirao K 2004 *J. Chem. Phys.* **120** 3297
[10] Huber K P and Herzberg G 1979 *Molecular Spectra and Molecular Structure*. Vol.4 *Constants of Diatomic Molecules* (New York: Van Nostrand Reinhold Company)
[11] Hofzumahaus A and Stuhl F 1985 *J. Chem. Phys.* **82** 5519
[12] Gaydon A G 1968 *Dissociation energies and Spectra of Diatomic Molecules* (London: Chapman and Hall)
[13] Raghavachari K, Trucks G W, Pople J A and Head-Gordon M 1989 *Chem. Phys. Lett.* **157** 479
[14] Dunning T H 1989 *J. Chem. Phys.* **90** 1007
[15] Kendall R A, Dunning T H and Harrison R J 1992 *J. Chem. Phys.* **96** 6796
[16] Woon D E and Dunning T H 1993 *J. Chem. Phys.* **98** 1358
[17] Sun J F, Zhang J C and Wang J M 2006 *Chin. Phys.* **15** 531
[18] Côté R, Dalgarno A and Jamieson M J 1994 *Phys. Rev.* A **50** 399
[19] Jamieson M J, Dalgarno A and Yukich J N 1992 *Phys. Rev.* A **46** 6956
[20] Frisch M J, Trucks G W, Schlegel H B, Scuseria G E, Robb M A, Cheeseman J R, Montgomery J A, Vreven T, Kudin K N, Burant J C, Millam J M, Iyengar S S, Tomasi J, Barone V, Mennucci B, Cossi M, Scalmani G, Rega N, Petersson G A, Nakatsuji H, Hada M, Ehara M, Toyota K, Fukuda R, Hasegawa J, Ishida M, Nakajima T, Honda Y, Kitao O, Nakai H, Klene M, Li X, Knox J E, Hratchian H P, Cross J B, Adamo C, Jaramillo J, Gomperts R, Stratmann R E, Yazyev O, Austin A J, Cammi R, Pomelli C, Ochterski J W, Ayala P Y, Morokuma K, Voth G A, Salvador P, Dannenberg J J, Zakrzewski V G, Dapprich S, Daniels A D, Strain M C, Farkas O, Malick D K, Rabuck A D, Raghavachari K, Foresman J B, Ortiz J V, Cui Q, Baboul A G, Clifford S, Cioslowski J, Stefanov B B, Liu G, Liashenko A, Piskorz P, Komaromi I, Martin R L, Fox D J, Keith T, Al-Laham M A, Peng C Y, Nanayakkara A, Challacombe M, Gill P M W, Johnson B, Chen W, Wong M W, Gonzalez C and Pople J A 2004 Gaussian 03 Revision D1 (Wallingford CT: Gaussian Inc.)
[21] Brazier C R, Ram R S and Bernath P F 1986 *J. Mol. Spectrosc.* **120** 381
[22] Boudjaadar D, Brion J, Chollet P, Guelachvili G and Vervoet M 1986 *J. Mol. Spectrosc.* **119** 352
[23] Malicet J, Brion J and Guenebaut H 1970 *J. Chim Phys.* **67** 25
[24] Murrell J N, Carter S, Farantos S C, Huxley P and Varandas J C 1984 *Molecular Potential Energy Functions* (Chichester: Wiley)
[25] Aguado A and Paniagua M 1992 *J. Chem. Phys.* **96** 1265
[26] Shi D H, Sun J F, Zhu Z L, Ma H, Liu Y F and Zhu Z H 2007 *Int. J. Quant. Chem.* **107** 1856
[27] Shi D H, Sun J F, Liu Y F, Ma H, Zhu Z L and Yang X D 2007 *Acta Phys. Sin.* **56** 4454 (in Chinese)
[28] Shi D H, Sun J F, Zhu Z L and Liu Y F 2007 *Chin. Phys.* **16** 2701
[29] Herzberg G 1951 *Molecular Spectra and Molecular Structure*, Vol.1 (New York: Van Nostrand-Reinhold)