Vol 16 No 10, October 2007
1009-1963/2007/16(10)/2962-06
Chinese Physics
© 2007 Chin. Phys. Soc.
and IOP Publishing Ltd

Investigations on spectroscopic parameters, vibrational levels, classical turning points and inertial rotation and centrifugal distortion constants for the $X^1\Sigma_g^+$ state of sodium dimer*

Yu Ben-Hai(余本海)[a)†], Dai Qi-Run(戴启润)[a)], Shi De-Heng(施德恒)[a)b)], and Liu Yu-Fang(刘玉芳)[b)]

[a)] *College of Physics and Electronic Engineering, Xinyang Normal University, Xinyang* 464000, *China*

[b)] *College of Physics and Information Engineering, Henan Normal University, Xinxiang* 453007, *China*

(Received 31 December 2006; revised manuscript received 1 February 2007)

The density functional theory (B3LYP, B3P86) and the quadratic configuration-interaction method including single and double substitutions (QCISD(T), QCISD) presented in Gaussian03 program package are employed to calculate the equilibrium internuclear distance R_e, the dissociation energy D_e and the harmonic frequency ω_e for the $X^1\Sigma_g^+$ state of sodium dimer in a number of basis sets. The conclusion is gained that the best R_e, D_e and ω_e results can be attained at the QCISD/6-311G(3df,3pd) level of theory. The potential energy curve at this level of theory for this state is obtained over a wide internuclear separation range from 0.16 to 2.0 nm and is fitted to the analytic Murrell–Sorbie function. The spectroscopic parameters D_e, D_0, R_e, ω_e, $\omega_e\chi_e$, α_e and B_e are calculated to be 0.7219 eV, 0.7135 eV, 0.31813 nm, 151.63 cm^{-1}, 0.7288 cm^{-1}, 0.000729 cm^{-1} and 0.1449 cm^{-1}, respectively, which are in good agreement with the measurements. With the potential obtained at the QCISD/6-311G(3df,3pd) level of theory, a total of 63 vibrational states is found when $J = 0$ by solving the radial Schrödinger equation of nuclear motion. The vibrational level, corresponding classical turning point and inertial rotation constant are computed for each vibrational state. The centrifugal distortion constants (D_v H_v, L_v, M_v, N_v and O_v) are reported for the first time for the first 31 vibrational states when $J = 0$.

Keywords: dissociation energy, vibrational level, turning point, centrifugal distortion constant
PACC: 3520G, 3640

1. Introduction

The potential energy curves (PECs) of alkali-metal dimers, especially the PEC for Na_2 ground state,[1−3] have received renewed interest in the past several years due to the discovery of Bose-Einstein condensation (BEC) in ultracold hydrogen,[4] lithium,[5] sodium,[6,7] potassium[8] and rubidium.[7] Detailed knowledge of PEC is very useful in the understanding of ultralow-energy collision processes between alkali-metal atoms since the relatively slow nuclear motion is very sensitive to the details of the electronic PEC.[9] In order to produce trustworthy dynamics, various cross sections and scattering lengths[10] at ultralow energies always need to use accurate PECs for calculations with a high accuracy.

Very recently, Taylor and Newman[11] have reported the PEC for the Na_2 ground state, which is in good agreement with measurements. In order to calculate the complete Na_2 ground-state PEC, they used the CCSD(T) method when the internuclear distance R is relatively small, and used the UCCSD(T) method when the R becomes relatively large since the energies via the CCSD(T) method are not convergent at larger values of R. Then, they combined the results from the two methods into a final one. And for this reason, the reliability of their PEC is greatly discounted. Furthermore, we have not found any complete calculations about the vibrational levels, classical turning points and inertial rotation and centrifugal distortion constants for this state, which are very useful in the theoretical computations of rovibrational transitions. Thus in this paper, we attempt to improve the ac-

*Project supported by the National Natural Science Foundation of China (Grant No 10574039), the Henan Innovation for University Prominent Research Talents (Grant No 2006KYCX002) and the Natural Science Foundation of Henan Province (Grant Nos 2006140008 and 2007140015).
†Corresponding author. E-mail: henanyubenhai@163.com

curacy of the *ab initio* potential. With the potential obtained here, we calculate the complete vibrational levels, classical turning points and inertial rotation and centrifugal distortion constants when J=0 for this state by solving the radial Schrödinger equation of nuclear motion. The present results are more complete than those available from previous investigations, which thus is symbolic of an improvement.

2. Methodological details

The calculations about the PEC for the Na_2 ground state are performed in Gaussian03 program package.[12] In calculations, we have used four kinds of theoretical methods, which include two kinds of density functional theories (B3LYP, B3P86) and two kinds of quadratic configuration-interaction methods (QCISD(T),QCISD). In addition, a number of basis sets, such as, Aug-cc-PVTZ, cc-PVTZ, 6-311++G(3df,3pd), 6-311++G(2df,2pd), 6-311++G(df,pd), 6-311G(3df,3pd), 6-311G(2df,2pd), 6-311++G(d,p), 6-311++G, 6-311G(df,pd), 6-311G(d,p), 6-311G and cc-PVQZ, are used. By comparison between the calculations and the measurements,[13] we find that the density functional theories (B3LYP, B3P86) can give rather accurate values of R_e and ω_e but much poor values of D_e; whereas the quadratic configuration-interaction methods (QCISD(T), QCISD) can give accurate values of D_e but relatively poor results of R_e and ω_e. By careful comparison with the measurements[13] about the D_e, ω_e and R_e, a most suitable basis set, 6-311G (3df,3pd),[14−16] and a most suitable method, QCISD,[12] are chosen. The computed D_e, ω_e and R_e results are listed in Table 1.

Table 1. Spectroscopic parameters for $Na_2(X^1\Sigma_g^+)$ at the QCISD/6-311G (3df,3pd) level of theory and the comparison with the available measurements.

source	D_e/eV	R_e/nm	ω_e/cm^{-1}	$\omega_e\chi_e$/cm^{-1}	B_e/cm^{-1}	α_e/cm^{-1}	D_0/eV
This work	0.7219	0.31813	151.63	0.7288	0.1449	0.000729	0.7135
Exp.[13]	0.7298	0.30790	159.12	0.7255	0.1547	0.000874	0.720

The PEC of this state is calculated at 0.02 nm intervals over the internuclear separation range from 0.16 to 2.0 nm at the QCISD/6-311G (3df,3pd) level of theory. The *ab initio* calculated points are fitted to the analytic Murrell–Sorbie (M-S) function with the least-squares fitting method. Thus the dissociation energy D_e and the analytic potential energy function (APEF) are attained. Based on the APEF obtained here, the force constants, quadratic f_2, cubic f_3 and quartic f_4, are determined. And then the spectroscopic parameters, $\omega_e\chi_e$, α_e and B_e, are calculated. And finally, using the APEF obtained at the QCISD/6-311G (3df,3pd) level of theory, the radial Schrödinger equation of nuclear motion is numerically solved to have all the vibrational levels and their classical turning points, R_{min} and R_{max}, the inertial rotation and centrifugal distortion constants when $J = 0$.

For the convenience of further calculations at this level of theory, we tabulate the computed potential energies $E(R)$ at selected values of the internuclear separation R as shows in Table 2 and depict the curve of the *ab initio* calculated points over this range in Fig.1.

Table 2. Potential energies $E(R)$ at different internuclear distances R for $Na_2(X^1\Sigma_g^+)$ at the QCISD/6-311G (3df,3pd) level of theory.

R/nm	$E(R)$/Hartree	R/nm	$E(R)$/Hartree	R/nm	$E(R)$/Hartree	R/nm	$E(R)$/Hartree
0.16	−323.58804	0.32	−323.71820	0.52	−323.69802	0.96	−323.69181
0.20	−323.66905	0.34	−323.71746	0.56	−323.69568	1.02	−323.69179
0.24	−323.70104	0.36	−323.71579	0.60	−323.69418	1.10	−323.69177
0.26	−323.70970	0.40	−323.71101	0.66	−323.69293	1.20	−323.69176
0.28	−323.71495	0.44	−323.70587	0.72	−323.69234	1.40	−323.69175
0.30	−323.71756	0.48	−323.70140	0.80	−323.69201	2.00	−323.69175

3. Results and discussion

The M-S function is a widely used potential energy function. It describes interaction potential energies of neutral diatomics well. The common M-S function is[17]

$$V(\rho) = -D_{\rm e}\Big(1 + \sum_{i=1}^{n} a_i \rho^i\Big)\exp(-a_1\rho), \qquad (1)$$

where $\rho = R - R_{\rm e}$, $R_{\rm e}$ is regarded as a fixed parameter in the fitting process, which is attained by the geometry optimization calculations in this paper. The parameters $D_{\rm e}$ and a_i are determined by the fitting method using the calculated *ab initio* data. Generally, satisfactory results can be obtained when n equals 3. Thus, Eq.(1) can be simplified into the following form:

$$V = -D_{\rm e}(1 + a_1\rho + a_2\rho^2 + a_3\rho^3)\exp(-a_1\rho). \qquad (2)$$

By iterating a system of normal equations based on a least-squares fitting, the parameters a_1,a_2, a_3 and $D_{\rm e}$ in Eq.(2) are fitted. The fitting results are listed in Table 3 together with the $R_{\rm e}$ value for integrality. At the same time, the fitting results over this internuclear separation range are intuitively shown in Fig.1, too.

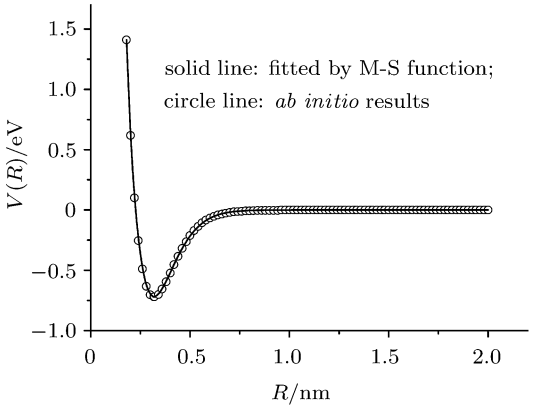


Fig.1. PEC of the ground state for sodium dimer.

Table 3. Parameters of M-S APEF for $Na_2(X^1\Sigma_g^+)$ at the QCISD/6-311G (3df,3pd) level of theory.

$D_{\rm e}$/eV	$R_{\rm e}$/nm	a_1/nm^{-1}	a_2/nm^{-2}	a_3/nm^{-3}	RMSE/eV
0.72193	0.31813	19.29788	116.35909	261.94042	1.6557×10^{-3}

In order to evaluate the fitting quality of PEC, we calculate the root-means-square error (RMSE),

$$\mathrm{RMSE} = \sqrt{\frac{1}{N}\Big[\sum_{i=1}^{N}(V_{\rm APEF} - V_{ab\ initio})^2\Big]}, \qquad (3)$$

where $V_{\rm APEF}$ and $V_{ab\ initio}$ are energies attained by the fitting and the *ab initio* calculations, respectively. N is the number of fitting points (here N = 93). The present RMSE is only 0.0016557 eV (about 0.038 kcal/mol). Obviously, our fitting accuracy about the APEF is greatly superior to the chemical accuracy (1.0 kcal/mol).[18] It shows that the analytic M-S function is very suitable for reproducing the PEC of this state, and the fitting process is of high quality. So, the present APEF collected in Table 3 should be credible and can be used to carry out the spectroscopic and vibrational manifold calculations, such as the spectroscopic parameters, the vibrational levels, the classical turning points, the inertial rotation and the centrifugal distortion constants, etc.

3.1. Spectroscopic parameters

Now, we calculate the spectroscopic parameters $B_{\rm e}$, $\alpha_{\rm e}$ and $\omega_{\rm e}\chi_{\rm e}$ of this state according to the APEF given in Table 3. Using Eq.(2), we can derive the expressions of the force constants f_2, f_3 and f_4 at the equilibrium position as follows:[19,20]

$$f_2 = D_{\rm e}(a_1^2 - 2a_2), \qquad (4)$$

$$f_3 = -6D_{\rm e}(a_3 - a_1a_2 + a_1^3/3, \qquad (5)$$

$$f_4 = D_{\rm e}(3a_1^4 - 12a_1^2a_2 + 24a_1a_3). \qquad (6)$$

Then the spectroscopic parameters $B_{\rm e}$, $\alpha_{\rm e}$ and $\omega_{\rm e}\chi_{\rm e}$ can be calculated according to the following Equations (7)–(9). The calculated results are listed in Table 1. From Table 1, one can easily find that the present values about $B_{\rm e}$, $\alpha_{\rm e}$ and $\omega_{\rm e}\chi_{\rm e}$ are in good agreement with the measurements.[13]

$$B_{\rm e} = \frac{h}{8\pi c\mu R_{\rm e}^2}, \qquad (7)$$

$$\alpha_{\rm e} = -\frac{6B_{\rm e}^2}{\omega_{\rm e}}\Big(\frac{f_3R_{\rm e}}{3f_2} + 1\Big), \qquad (8)$$

$$\omega_{\rm e}\chi_{\rm e} = \frac{B_{\rm e}}{8}\Big[-\frac{f_4R_{\rm e}^2}{f_2} + 15\Big(1 + \frac{\omega_{\rm e}\alpha_{\rm e}}{6B_{\rm e}^2}\Big)^2\Big]. \qquad (9)$$

3.2. Vibrational manifolds

A more stringent way to compare the *ab initio* results with the measurements is to attempt to reproduce the Rydberg–Klein–Rees (RKR) data: the

vibrational levels and corresponding classical turning points. Only in that way can it be clearly demonstrated whether the present APEF accurately describes the PEC for the Na_2 ground state. In order to attain the vibrational levels of this state, we must solve the following radial Schrödinger equation of nuclear motion in the adiabatic approximation,

$$\left[-\frac{\hbar^2}{2\mu}\frac{\mathrm{d}^2}{\mathrm{d}r^2}+\frac{\hbar^2}{2\mu r^2}J(J+1)+V(r)\right]\Psi_{\nu.J}(r) = E_{\nu,J}\,\Psi_{\nu.J}(r). \tag{10}$$

Here, $V(r)$ is the adiabatic rotationless APEF given in Table 3; ν and J are the vibrational and rotational quantum numbers, respectively; μ is the reduced mass of molecule Na_2. The rotational sublevel of a given vibrational level is represented by the following power series,[21]

$$E_{\nu,J} = G(v) + B_v[J(J+1)] - D_v[J(J+1)]^2 + H_v[J(J+1)]^3 + L_v[J(J+1)]^4 + M_\nu[J(J+1)]^5 + N_\nu[J(J+1)]^6. \tag{11}$$

By solving Eq.(10) numerically, we can obtain a total of 63 vibrational states for the Na_2 ground state when $J = 0$. For each vibrational state, 1 vibrational level $G(\nu)$ and corresponding classical turning points, $R_{\max}$ and $R_{\min}$, 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 attained. Here, all the 63 vibrational levels, their corresponding classical turning points and inertial rotation constants are given in Table 4, and the 6 centrifugal distortion constants of the first 31 vibrational states are shown in Table 5.

Table 4. Vibrational levels, classical turning points and initial rotation constants of $Na_2(X^1\Sigma_g^+)$ at the QCISD/6-311G (3df,3pd) level of theory when $J = 0$.

υ	$G(\upsilon)/\mathrm{cm}^{-1}$	$R_{\min}$/nm	$R_{\max}$/nm	$B_\upsilon/\mathrm{cm}^{-1}$	υ	$G(\upsilon)/\mathrm{cm}^{-1}$	$R_{\min}$/nm	$R_{\max}$/nm	$B_\upsilon/\mathrm{cm}^{-1}$
0	76.987	0.30489	0.32250	0.1445451	32	4152.174	0.23690	0.50334	0.1100138
1	229.972	0.29582	0.34384	0.1438126	33	4248.313	0.23613	0.50892	0.1084450
2	381.479	0.28987	0.35212	0.1430623	34	4342.234	0.23539	0.51463	0.1068339
3	531.493	0.28519	0.35915	0.1422938	35	4433.896	0.23467	0.52050	0.1051784
4	680.001	0.28127	0.36548	0.1415070	36	4523.259	0.23398	0.52652	0.1034764
5	826.987	0.27785	0.37135	0.1407013	37	4610.282	0.23332	0.53273	0.1017254
6	972.436	0.27480	0.37689	0.1398765	38	4694.919	0.23269	0.53913	0.0999228
7	1116.333	0.27204	0.38220	0.1390321	39	4777.124	0.23208	0.54575	0.0980656
8	1258.661	0.26952	0.38731	0.1381677	40	4856.848	0.23150	0.55260	0.0961507
9	1399.404	0.26718	0.39229	0.1372829	41	4934.041	0.23094	0.55972	0.0941743
10	1538.544	0.26501	0.39716	0.1363774	42	5008.647	0.23040	0.56712	0.0921323
11	1676.064	0.26297	0.40194	0.1354506	43	5080.609	0.22989	0.57485	0.0900201
12	1811.945	0.26106	0.40665	0.1345021	44	5149.867	0.22941	0.58294	0.0878324
13	1946.170	0.25926	0.41132	0.1335315	45	5216.355	0.22894	0.59144	0.0855631
14	2078.718	0.25755	0.41595	0.1325381	46	5280.005	0.22850	0.60039	0.0832054
15	2209.570	0.25593	0.52056	0.1315216	47	5340.744	0.22808	0.60987	0.0807511
16	2338.705	0.25439	0.42515	0.1304813	48	5398.491	0.22770	0.61994	0.0781907
17	2466.104	0.25292	0.42974	0.1294167	49	5453.161	0.22733	0.63072	0.0755131
18	2591.743	0.25152	0.43433	0.1283271	50	5504.662	0.22698	0.64230	0.0727047
19	2715.602	0.25018	0.43894	0.1272120	51	5552.893	0.22666	0.65484	0.0697492
20	2837.656	0.24890	0.44357	0.1260706	52	5597.742	0.22637	0.66855	0.0666262
21	2957.883	0.24767	0.44822	0.1249023	53	5639.088	0.22609	0.68368	0.0633101
22	3076.258	0.24648	0.45291	0.1237063	54	5676.792	0.22584	0.70060	0.0597677
23	3192.756	0.24535	0.45764	0.1224817	55	5710.700	0.22563	0.71983	0.0559546
24	3307.350	0.24426	0.46242	0.1212278	56	5740.636	0.22543	0.74215	0.0518091
25	3420.015	0.24321	0.46726	0.1199435	57	5766.394	0.22527	0.76885	0.0472406
26	3530.722	0.24221	0.47216	0.1186280	58	5787.728	0.22513	0.80221	0.0421047
27	3639.443	0.24124	0.47713	0.1172802	59	5804.335	0.22502	0.84693	0.0361425
28	3746.148	0.24030	0.48218	0.1158990	60	5815.819	0.22495	0.91572	0.0287739
29	3850.806	0.23940	0.48732	0.1144830	61	5819.600	0.22492	0.97533	0.0196018
30	3953.386	0.23854	0.49255	0.1130312	62	5822.030	0.22491	1.19817	0.0153207
31	4053.853	0.23770	0.49789	0.1115419					

The experimental results about the vibrational levels, classical turning points and inertial rotation constants can be found in the recent literature.[22] For the sake of clarity of this paper, we do not tabulate these measurements here. When we compare the present results with these measurements,[22] we can clearly see that they are in good agreement with each other. Therefore, we say that the present APEF obtained at the QCISD/6-311G (3df,3pd) level of theory well describes this ground state.

Unfortunately, we have not found any complete experimental results about the 6 centrifugal distortion constants (D_ν, H_ν, L_ν, M_ν, N_ν and O_ν) for the Na_2 ground state to the best of our knowledge. Thus we cannot make any direct complete comparison with measurements. But according to the high-quality fitting process of this APEF, the good agreement between the present spectroscopic parameters and the measurements[13] and between the present vibrational levels and the experimental results,[22] we have reasons to believe that the results collected in Tables 5 are accurate.

Table 5. Six centrifugal distortion constants of the first 31 vibrational states for $Na_2(X^1\Sigma_g^+)$ from the QCISD/6-311G (3df,3pd) level of theory when $J = 0$.

υ	$D_\upsilon/10^{-7}$ cm^{-1}	$H_\upsilon/10^{-12}$ cm^{-1}	$L_\upsilon/10^{-17}$ cm^{-1}	$M_\upsilon/10^{-22}$ cm^{-1}	$N_\upsilon/10^{-27}$ cm^{-1}	$O_\upsilon/10^{-32}$ cm^{-1}
0	5.1326224	2.0321581	−1.9178064	1.5766648	−1.7663118	1.7835832
1	5.1940357	2.0593765	−1.9779657	1.6133477	−1.8269628	1.8138441
2	5.2557235	2.0845518	−2.0377509	1.6451256	−1.8835288	1.8325250
3	5.3177221	2.1075564	−2.0972130	1.6716793	−1.9369470	1.8194567
4	5.3800723	2.1282557	−2.1564490	1.6925590	−1.9869135	1.7701631
5	5.4428202	2.1465097	−2.2155632	1.7074043	−2.0347942	1.6439415
6	5.5060172	2.1621694	−2.2747143	1.7156660	−2.0798285	1.4552114
7	5.5697210	2.1750788	−2.3340637	1.7169929	−2.1251611	1.1003181
8	5.6339953	2.1850686	−2.3938577	1.7106282	−2.1679738	0.6801844
9	5.6989109	2.1919609	−2.4543405	1.6961134	−2.2120094	0.0731283
10	5.7645460	2.1955632	−2.5158163	1.6728573	−2.2604817	−0.851630
11	5.8309865	2.1956646	−2.5786768	1.6398807	−2.3109417	−1.950427
12	5.8983273	2.1920375	−2.6433571	1.5962515	−2.3643686	−3.188843
13	5.9666726	2.1844366	−2.7103169	1.5413863	−2.4325056	−5.135486
14	6.0361367	2.1725859	−2.7801793	1.4737111	−2.5107026	−7.433632
15	6.1068452	2.1561839	−2.8536256	1.3918700	−2.6034725	−10.20689
16	6.1789359	2.1348962	−2.9314485	1.2941369	−2.7140027	−13.42936
17	6.2525599	2.1083503	−3.0145671	1.1786080	−2.8494877	−17.32007
18	6.3278833	2.0761300	−3.1040509	1.0427891	−3.0142114	−21.77114
19	6.4050883	2.0377679	−3.2011413	0.8840082	−3.2204845	−27.25761
20	6.4843722	1.9926916	−3.3085537	0.6773872	−3.1741142	−2.420025
21	6.5659611	1.9403903	−3.4256355	0.4581618	−3.4409148	−3.260806
22	6.6500950	1.8801466	−3.5554918	0.2027511	−3.7778692	−4.279251
23	6.7370416	1.8111893	−3.7004688	−0.095148	−4.2031579	−5.520625
24	6.8270966	1.7326366	−3.8633356	−0.443279	−4.7397935	−7.049829
25	6.9205877	1.6434766	−4.0473730	−0.851202	−5.4169541	−8.949051
26	7.0178779	1.5425440	−4.2564843	−1.330773	−6.2720054	−11.32704
27	7.1193711	1.4284915	−4.4953340	−1.896762	−7.3530770	−14.34191
28	7.2255175	1.2997556	−4.7695234	−2.567684	−8.7225087	−18.18891
29	7.3368201	1.1545145	−5.0858135	−3.366863	−10.461778	−23.14565
30	7.4538429	0.9906369	−5.4524091	−4.323866	−12.678054	−29.58454

4. Conclusions

In this paper, the equilibrium internuclear distance, the dissociation energy and the harmonic frequency for the Na_2 ground state have been calculated using the density functional theory (B3LYP, B3P86) and the quadratic configuration-interaction method

including single and double substitutions (QCISD(T), QCISD) presented in Gaussian03 program package in a number of basis sets. And the QCISD/6-311G (3df,3pd) level of theory is determined to be the best one by comparing the calculations with the measurements.[13] With the potential obtained at the QCISD/6-311G (3df,3pd) level of theory, a total of 63 vibrational states are found by solving the radial Schrödinger equation of nuclear motion. The complete vibrational levels, classical turning points and inertial rotation constants are also calculated for each vibrational state. Favourable agreement has been found by comparing our calculations with the measurements.[22] In addition, we have further computed six centrifugal distortion constants for this state when $J = 0$ for the first time. The results at present are more complete than those available from previous investigations, which thus is symbolic of an improvement. As a further investigation, we will employ our derived analytic PEFs to calculate the various cross sections,[23,24] especially at very low energies.

References

[1] Matsunaga N and Zavitsas A A 2004 *J. Chem. Phys.* **120** 5624 and references herein

[2] Gutowski M 1999 *J. Chem. Phys.* **110** 4695

[3] Matsunaga N, Rogers D W and Zavitsas A A 2003 *J. Org. Chem.* **68** 3158

[4] Fried D G, Killian T C, Willmann L, Landhuis D, Moss S C, Kleppner D and Greytal T S 1998 *Phys. Rev. Lett.* **81** 3811

[5] Bradley C C, Sackett C A and Hulet R G 1997 *Phys. Rev. Lett.* **78** 985

[6] Davis K B, Mewes M -O, Andrews M R, Van Druten N J, Durfee D S, Kurn D M and Ketterle W 1995 *Phys. Rev. Lett.* **75** 3969

[7] Dalfovo F, Giorgini S, Pitaevskii L P and Stringari S 1999 *Rev. Mod. Phys.* **71** 463

[8] Côté R, Dalgarno A and Wang H 1998 *Phys. Rev.* A **57** 4118

[9] Yan S Y 2006 *Acta Phys. Sin.* **55** 3408 (in Chinese)

[10] Shi D H, Sun J F, Zhu Z L and Liu Y F 2007 *Chin. Phys.* **16** 1655

[11] Taylor B K and Newman P R 2003 *J. Chem. Phys.* **118** 8770

[12] Frisch M J, Trucks G W, Schlegel H B, Scuseria G E, Robb M A, Cheeseman J R, Jr 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 2003 Gaussian03 Revision A2 (Pittsburgh PA: Gaussian Inc.)

[13] Huber K P and Herzberg G 1979 *Molecular Spectra and Molecular Structure* Vol.4 *Constants of Diatomic Molecules* (New York: Van Nostrand Reinhold) p432

[14] Krishnan R, Binkley J S, Seeger R and Pople J A 1980 *J. Chem. Phys.* **72** 650

[15] McLean A D and Chandler G S 1980 *J. Chem. Phys.* **72** 5639

[16] Frisch M J, Pople J A and Binkley J S 1984 *J. Chem. Phys.* **80** 3265

[17] Murrell J N, Carter S, Farantos S C, Huxley P and Varandas J C 1984 *Molecular Potential Energy Functions* (Chichester: John Wiley & Sons) p9

[18] Aguado A and Paniagua M 1992 *J. Chem. Phys.* **96** 1265

[19] Shi D H, Liu Y F, Sun J F, Yang X D and Zhu Z L 2006 *Chin. Phys.* **15** 1015

[20] Shi D H, Liu Y F, Sun J F, Zhu Z L and Yang X D 2006 *Chin. Phys.* **15** 2928

[21] Herzberg G 1951 *Molecular Spectra and Molecular Structure* Vol.1 (New York: Van Nostrand Reinhold)

[22] Rabitz T –S Ho and Scoles G 2000 *J. Chem. Phys.* **112** 6218

[23] Shi D H, Sun J F, Zhu Z L, Liu Y F and Yang X D 2005 *Acta Phys. Sin.* **54** 3548 (in Chinese)

[24] Shi D H, Sun J F, Liu Y F, Ma H and Zhu Z L 2006 *Acta Phys. Sin.* **55** 4096 (in Chinese)