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Oscillator strengths for $2\,^2S$–n^2P transitions of the lithium isoelectronic sequence from $Z = 11$ to 20*

Hu Mu-Hong(胡木宏) and Wang Zhi -Wen(王治文)†

School of Physics and Electronic Technology, Liaoning Normal University, Dalian 116029, *China*

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The dipole-length, dipole-velocity and dipole-acceleration absorption oscillator strengths for the $1s^22s$–$1s^2np$ ($3 \leq n \leq 9$) transitions of lithium-like systems from $Z = 11$ to 20 are calculated by using the energies and the multi-configuration interaction wave functions obtained from a full core plus correlation method, in which relativistic and mass-polarization effects on the energy, as the first-order perturbation corrections, are included. The results of three forms are in good agreement with each other, and closely agree with the experimental data available in the literature. Based on the quantum defects obtained with quantum defect theory (QDT), the discrete oscillator strengths for the transitions from the ground state to highly excited states $1s^2np$ ($n \geq 10$) and oscillator strength densities corresponding to the bound-free transitions are obtained for these ions.

Keywords: lithium isoelectronic sequence, oscillator strengths, quantum defect
PACC: 3130, 3110, 3270

1. Introduction

The study of transition rates or oscillator strengths for highly ionized atomic systems has been a subject of considerable interest for many important fields, such as astrophysics, controlled thermonuclear reactions, etc. From the theoretical viewpoint, to obtain accurate transition rates or oscillator strengths, accurate wave functions have to be used for both the initial and final states. Unlike the calculation of energy where high precision results can be obtained, the lack of a bound property makes a precision calculation of the transition rates or oscillator strengths very challenging. For helium- and lithium-like ions, accurate non-relativistic calculated results have been presented by Kono and Hattori,[1] Cann and Thakkar,[2] and by Drake.[3] More recently, the oscillator strengths for $2s^2S$–$2p^2P$ transitions of the lithium isoelectronic sequence up to $Z = 20$ were calculated by Yan, Tambasco and Drake.[4] On the other hand, theoretical research of this important spectral property along an isoelectronic sequence is of significance, because it is useful to test the reliability of the theoretical method and to determine the variation regularities of varies physical effects with increasing nuclear charge Z in the systems along the sequence.

Recently an elegant and complete variational approach, named the full-core plus correlation (FCPC) method,[5] has been extended to calculate the transition energies, oscillator strengths and fine-structure splittings for lithium-like ions with larger Z, and the calculated results are very satisfactory.[6−16] As we know, reliable theoretical prediction on the oscillator strength is particularly important because high precision measurements are difficult to carry out. In *ab initio* calculations, the quality of the results is usually judged by the agreement of the dipole-length, -velocity and -acceleration oscillator strengths. This is because the operators in these three formulas give different weights to different parts of the configuration space. The dipole-acceleration formula, in particular, weights heavily the part of configuration space which is close to the nucleus. It is usually difficult to find an accurate wave function in this region using a variation method. For three-electron systems, the results obtained from acceleration formula could differ from the dipole-length and dipole-velocity results by several orders of magnitude.[17]

In this paper, the dipole-length, dipole-velocity and dipole-acceleration absorption oscillator strengths of the $1s^22s$–$1s^2np$ ($3 \leq n \leq 9$) transitions for the lithium isoelectronic sequence from $Z = 11$ to 20 are

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†Corresponding author. E-mail: zh.w.wang@163.com

calculated by using an approximation with the first order of relativistic correction. The relativistic quantum defects, as functions of energy, of $1s^2np$ series are determined, and our theoretical predictions on the oscillator strength of these ions are extrapolated to their whole energy regions by combining with the quantum defect theory (QDT).

2. Theory

The total wave functions of the lithium-like systems with $1s^2$-core used in this paper can be written as

$$\Psi(1,2,3) = A\left[\Phi_{1s1s}(1,2)\sum_i d_i r_3^i \mathrm{e}^{-\beta r_3} Y_{l(i)}(3)\chi(3) + \sum_i C_i \Phi_{n(i),l(i)}(1,2,3)\right]. \quad (1)$$

Here A is an antisymmetrization operator. The first term on the right-hand side of Eq.(1) is the product of a predetermined $1s^2$-core wave function $\Phi_{1s1s}(1, 2)$ and a linear combination of Slater orbitals for the valence electron, and describes the electron correlation in $1s^2$-core and the effect of the valence electron in a three-electron system. The second term is similar to the expansion in terms of the basis set in the traditional CI method, and describes the relaxation of $1s^2$-core and the other possible correlations in the three-electron system. The expressions of $\Phi_{1s1s}(1, 2)$ and $\Phi_{n(i),l(i)}(1, 2, 3)$ in Eq.(1) can be found in Ref.[5]. In the $1s^22s$–$1s^2np$ transitions of lithium-like systems, the $1s^2$-core behaves like a spectator, so the FCPC wave functions (1) could be very effectively used to calculate[9−11] the dipole-oscillator strengths for the $1s^22s$–$1s^2np$ ($3 \le n \le 9$) transitions of lithium-like ions from $Z = 11$ to 20.

The oscillator strength from an initial state i to a final state j can be given by any of the following three forms[18]

$$f_{\mathrm{L}} = \frac{2}{3}(E_j - E_i)|\langle \Psi_i|\boldsymbol{r}|\Psi_j\rangle|^2, \quad (2a)$$

$$f_{\mathrm{V}} = \frac{2}{3}(E_j - E_i)^{-1}|\langle \Psi_i|\nabla|\Psi_j\rangle|^2, \quad (2b)$$

$$f_{\mathrm{A}} = \frac{2}{3}(E_j - E_i)^{-3}|\langle \Psi_i|\frac{\boldsymbol{r}}{r^3}|\Psi_j\rangle|^2, \quad (2c)$$

where f_{L}, f_{V}, and f_{A} separately denote the oscillator strength in length, velocity, and acceleration forms. E_i and E_j are the energies of the initial and final states for the dipole transition, respectively. In the calculations of the energies, the contributions from relativistic and mass-polarization effects are included by the use of perturbation theory.[9,11] These three alternatives are equivalent theoretically when exact wave functions are employed. But, as mentioned previously, they usually give rather different results when approximate wave functions are used. To a great extent, whether the f-values obtained from the three formulas are in agreement with each other becomes a rigorous evaluation of the quality for the wave functions used, and the reliability of the f-values obtained in calculations.

It is known that the oscillator strength densities corresponding to the final states in the continuum are associated with the discrete oscillator strength corresponding to the bound-bound transitions.[19] Thus the oscillator strength densities of the bound-bound transitions can be defined as

$$\tau(E) = \frac{(n^*)^3}{Z^2} f_{ij} \quad \text{(in a.u.)}. \quad (3)$$

Here E is the energy of the final state, Z is the charge of the ion core, and f_{ij} is the discreet oscillator strength. n^* is the effective principal quantum number for the final state, which can be determined from the following formula according to the relativistic QDT[19]

$$E_{nk} = mc^2\left\{\frac{1}{[1+(Z\alpha/n^*)^2]^{1/2}} - 1\right\}, \quad (4)$$

where E_{nk} is the energy obtained from the FCPC method, α is the fine-structure constant, and mc^2 is the rest energy of the electron (in atomic units, $mc^2 = \alpha^{-2}$). The relationship between the effective principal quantum number n^* and the relativistic quantum defect μ_{rel} is given by[19]

$$\mu_{\mathrm{rel}} = n - n^* + \gamma - |k|, \quad (5)$$

where $\gamma = [k^2 - (\alpha Z)^2]^{1/2}$. If $j = l+1/2$, $k = -(l+1)$, and if $j = l - 1/2$, $k = l$.

For highly excited $1s^2np$ states with the principal quantum number $n \ge 10$, the relativistic quantum defect μ_{rel} should be a smooth function of energy and could be approximated by a weakly varying function of energy in the following form

$$\mu_{\mathrm{rel}}(E_{nk}) = \mu_0 + h_1 E_{nk} + h_2 E_{nk}^2. \quad (6)$$

The coefficients μ_0, h_1, and h_2 for this series are determined by using the $\mu_{\rm rel}$ values calculated from Eqs.(4) and (5). Treating Eqs.(4) and (6) as a set of equations for E_{nk} and $\mu_{\rm rel}$, the quantum defect $\mu_{\rm rel}$ and the energy E_{nk} for highly excited states ($n \geq 10$) can be determined by an iteration method.

In the limit $E \rightarrow I$ (from below), where I is the ionization potential of the system, the oscillator strength densities of the bound-bound transitions $\tau(E)$, as a function of E, will match to the oscillator strength densities, $\mathrm{d}f/\mathrm{d}\varepsilon$, of continuum states, namely

$$\tau(E) = \frac{(n^*)^3}{Z^2} f_{ij} = \frac{\mathrm{d}f}{\mathrm{d}\varepsilon}. \quad (7)$$

As far as the $1s^22s$–$1s^2np$ transition of lithium-like systems is concerned, the Cooper minimum and the following maximum are not found in the near-threshold energy region.[20] Hence, the discreet oscillator strength f_{ij} below the threshold in Eq.(7) can be extrapolated to the oscillator strength densities, $\mathrm{d}f/\mathrm{d}\varepsilon$, above the threshold. In the near-threshold region ($|E| \leq I/2$), the oscillator strength and the oscillator strength densities can be accurately approximated by the following form[21]

$$\tau(E) = \frac{(n^*)^3}{Z^2} f_{ij} = \frac{\mathrm{d}f}{\mathrm{d}\varepsilon} = \left[\frac{E_i}{E_i - E_j}\right]^S \left.\frac{\mathrm{d}f}{\mathrm{d}\varepsilon}\right|_{\varepsilon=0}. \quad (8)$$

Here the coefficient s and the oscillator strength densities at the threshold, $\mathrm{d}f/\mathrm{d}\varepsilon|_{\varepsilon=0}$, can be determined from the discreet oscillator strengths obtained from FCPC method. In this paper, s is a fitting parameter, and should be a function of Z. Equations (3) and (8) make it possible to determine the oscillator strength for the transition from initial state, $1s^22s$, to all the finial states of the $1s^2np$ Rydberg series, including continuum states.

3. Results and discussion

In most cases, a transition process in the atomic system only involves the participation of one or two electrons; the rest of the electrons acts as spectators.[18] In principle, one may compromise on the accuracy of the part of the wave function for the spectator as long as they are the same in the initial and final states. However, one must make sure that the part of the wave function for the active electron used in calculation is sufficiently accurate. In fact, the theoretical method adapted in this paper appropriately meets this requirement. So we have reason to believe that our theoretical prediction on the oscillator strengths of lithium-like ions obtained in this paper should be accurate and reliable.

The energies of initial and final states for the transitions in Eqs.(2a)–(2c) are determined by the summation of the non-relativistic energies and the first order of relativistic corrections (including mass-polarization correction).[9,11] This means that the results calculated from these three formulas can be considered as relativistic oscillator strengths to the extent of the first-order approximation.

The oscillator strengths in three forms for the $1s^22s$–$1s^2np$ ($3 \leq n \leq 9$) transitions of lithium-like ions from Na IX to Ca XVIII are listed in Table 1. As can be seen, the agreement between the oscillator strengths from the length and velocity forms is up to three or four digits in most cases, and the acceleration results agree closely with the length and velocity results too. The experimental data available in the literature[22] are also listed in Table 1 for comparison. To our knowledge, there are no experiment data for the cases of $n = 3$, 8, and 9 yet. It appears that the agreement of our oscillator strengths with them is satisfactory. As pointed out previously, equations (2a)–(2c) are sensitive to the accuracy of the wave functions in different regions of configuration space, respectively. Our results seem to suggest that our FCPC wave functions should be accurate in the whole space from the region close to the nucleus to the large-r region, and the f-values obtained in this paper are reliable. The variation of the length-f values for $1s^22s$–$1s^2np$ ($3 \leq n \leq 9$) transitions with increasing Z along this sequence is shown in Fig.1. Our calculated f-values agree closely with experimental data available in the literature. The f-values slowly increase with increasing Z from $Z = 11$ to 20. The variation of relativistic correction, to the extent of the first-order approximation, to oscillator strengths for $1s^22s$–$1s^23p$ transitions with Z is shown in Fig.2. This correction, which is the difference between the results listed in Table 1 and corresponding non-relativistic f-values, increases monotonically with increasing Z along this sequence. For other transitions, similar regularity is also found. For a given ion, the f-values decrease with increasing n along the Rydberg series of final states $1s^2np$. As an example, figure 3 gives the variation of the f-values for $1s^22s$–$1s^2np_{3/2}$ and $1s^22s$–$1s^2np_{1/2}$ transitions with increasing n in Cl XV.

Table 1. The oscillator strength of $1s^2 2s$–$1s^2 np$ ($3 \le n \le 9$) transitions for lithium-like systems from $Z = 11$ to 20.

Z		$3p$	$4p$	$5p$	$6p$	$7p$	$8p$	$9p$
11	$f_{\rm L}$	0.31501	0.08349	0.03538	0.01857	0.01104	0.00714	0.00491
	$f_{\rm V}$	0.31351	0.08312	0.03524	0.01850	0.01100	0.00711	0.00489
	$f_{\rm A}$	0.31261	0.08297	0.03515	0.01845	0.01094	0.00707	0.00488
	exp.		0.088	0.0373	0.0197	0.0116		
12	$f_{\rm L}$	0.32588	0.08543	0.03607	0.01890	0.01123	0.00725	0.00498
	$f_{\rm V}$	0.32395	0.08503	0.03590	0.01882	0.01118	0.00722	0.00496
	$f_{\rm A}$	0.32261	0.08462	0.03572	0.01871	0.01113	0.00717	0.00486
	exp.		0.089	0.0379	0.02	0.0118		
13	$f_{\rm L}$	0.33503	0.08704	0.03666	0.01916	0.01137	0.00734	0.00499
	$f_{\rm V}$	0.33264	0.08654	0.03644	0.01907	0.01132	0.00731	0.00497
	$f_{\rm A}$	0.33091	0.08597	0.03619	0.01893	0.01123	0.00725	0.00496
	exp.		0.092	0.0384	0.0202	0.0119		
14	$f_{\rm L}$	0.34287	0.08841	0.03711	0.01940	0.01151	0.00742	0.00507
	$f_{\rm V}$	0.34006	0.08781	0.03687	0.01928	0.01144	0.00738	0.00504
	$f_{\rm A}$	0.33720	0.08715	0.03661	0.01915	0.01137	0.00732	0.00501
	exp.		0.094	0.0388	0.0204	0.012		
15	$f_{\rm L}$	0.34966	0.08956	0.03752	0.01960	0.01162	0.00749	0.00512
	$f_{\rm V}$	0.34634	0.08887	0.03724	0.01945	0.01154	0.00744	0.00509
	$f_{\rm A}$	0.34323	0.08810	0.03693	0.01929	0.01143	0.00741	0.00507
	exp.		0.095	0.0391	0.0205	0.0121		
16	$f_{\rm L}$	0.35563	0.09057	0.03788	0.01976	0.01171	0.00756	0.00520
	$f_{\rm V}$	0.35176	0.08977	0.03755	0.01960	0.01162	0.00750	0.00516
	$f_{\rm A}$	0.34788	0.08894	0.03723	0.01943	0.01151	0.00748	0.00507
	exp.		0.095	0.0394	0.0207	0.0122		
17	$f_{\rm L}$	0.36093	0.09141	0.03821	0.01992	0.01180	0.00760	0.00528
	$f_{\rm V}$	0.35646	0.09054	0.03782	0.01972	0.01169	0.00753	0.00523
	$f_{\rm A}$	0.35198	0.08960	0.03744	0.01952	0.01157	0.00745	0.00517
	exp.		0.096	0.0397	0.0208	0.0122		
18	$f_{\rm L}$	0.36565	0.09232	0.03844	0.02002	0.01186	0.00766	0.00527
	$f_{\rm V}$	0.36054	0.09120	0.03804	0.01983	0.01175	0.00759	0.00521
	$f_{\rm A}$	0.35555	0.09018	0.03764	0.01962	0.01163	0.00749	0.00503
	exp.		0.097	0.0398	0.0208	0.0122		
19	$f_{\rm L}$	0.36995	0.09296	0.03870	0.02016	0.01194	0.00769	0.00521
	$f_{\rm V}$	0.36413	0.09178	0.03825	0.01992	0.01180	0.00760	0.00515
	$f_{\rm A}$	0.35833	0.09054	0.03777	0.01967	0.01165	0.00751	0.00509
	exp.		0.097	0.0399	0.0209	0.0123		
20	$f_{\rm L}$	0.37384	0.09363	0.03893	0.02026	0.01199	0.00777	0.00527
	$f_{\rm V}$	0.36730	0.09229	0.03841	0.02000	0.01184	0.00767	0.00521
	$f_{\rm A}$	0.35735	0.09094	0.03787	0.01973	0.01169	0.00759	0.00515
	exp.		0.098	0.04	0.021	0.0123		

* The experiment data in this table are from Ref.[22].

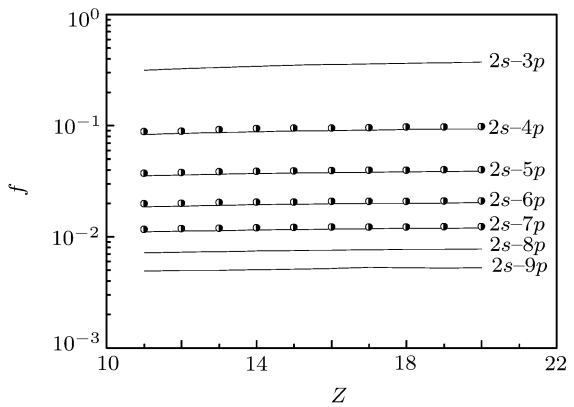


Fig.1. Length oscillator strengths of $1s^2 2s$–$1s^2 np$ transitions for the lithium isoelectronic sequence. The dots represent experimental data.[22] The solid curves represent our calculated results.

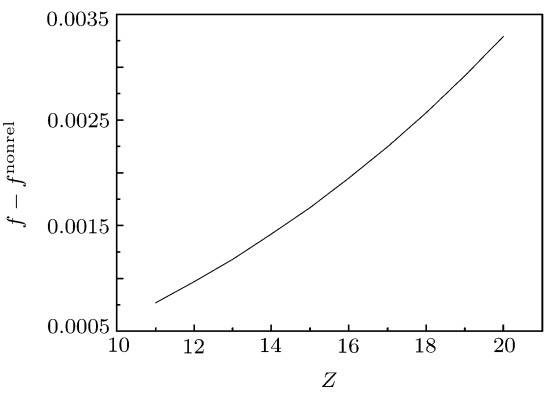


Fig.2. The variation of relativistic corrections to oscillator strengths of $1s^2 2s$–$1s^2 3$p transitions with increasing Z.

Equations (3) and (8) make it possible to easily determine oscillator strengths for transitions from the same initial state to all the states of the Rydberg series. The oscillator strength densities, $\mathrm{d}f/\mathrm{d}\varepsilon|_{\varepsilon=0}$, at threshold $E = I$ and the fitting parameter s in Eq.(8) are listed in Table 2. Figure 4 depicts oscillator strengths of $1s^2 2s$–$1s^2 np$ transitions in the whole energy regions for the sequence. The solid curves in the figure are obtained from Eqs.(3) and (8). It is seen from this figure that the discrete oscillator strengths calculated from the FCPC energies and wave functions lie rather well along the curves, and at the threshold $E = I$ the discrete oscillator strengths for the transitions from the same initial state $1s^2 2s$ to highly excited states $1s^2 np$ do smoothly adjoin the oscillator strength densities to corresponding continuum states for these ions. It suggests that our procedure should be reasonable and the results of our extrapolation are reliable and accurate.

Table 2. The oscillator strength density, $\mathrm{d}f/\mathrm{d}\varepsilon|_{\varepsilon=0}$, at the threshold and the s value in equation (8).

Z	11	12	13	14	15
$\mathrm{d}f/\mathrm{d}\varepsilon\|_{\varepsilon=0}$	0.04136	0.03396	0.02836	0.02405	0.02064
s	1.69	1.72	1.74	1.76	1.77
Z	16	17	18	19	20
$\mathrm{d}f/\mathrm{d}\varepsilon\|_{\varepsilon=0}$	0.01790	0.01565	0.01385	0.01230	0.01101
s	1.78	1.80	1.80	1.81	1.82

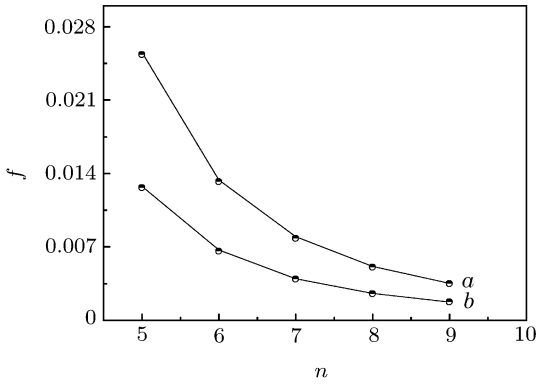


Fig.3. The variation of oscillator strengths of $1s^2 2s$–$1s^2 np$ ($5 \le n \le 9$) transitions with increasing n in Cl XV. Curve a: $1s^2 2s$–$1s^2 np_{3/2}$ transitions; curve b: $1s^2 2s$–$1s^2 np_{1/2}$ transitions. The dots represent the f-values computed from the full core plus correlation method.

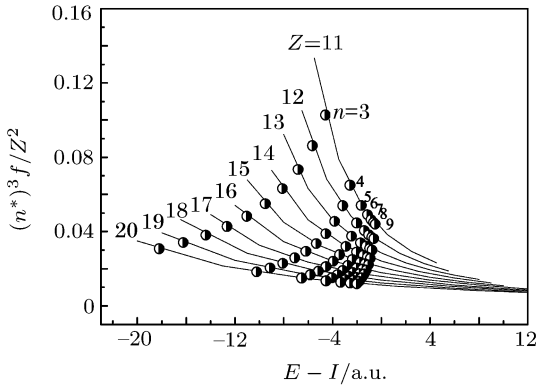


Fig.4. Oscillator strengths of $1s^2 2s$–$1s^2 np$ ($3 \le n \le 9$) transitions for the sequence. The solid curves are obtained from Eqs.(3) and (8), and the dots represent the values computed from Eq.(3). The discrete oscillator strengths are multiplied by the respective factors $(n^*)^3/Z^2$. The continuum oscillator strengths above the threshold are $\mathrm{d}f/\mathrm{d}\varepsilon$. The numbers beside the curve on the right side represent n-values of active electrons in the final states $1s^2 np$.

4. Summary

In this work, the relativistic dipole absorption oscillator strengths for $1s^2 2s$–$1s^2 np$ transition of the lithium isoelectronic sequence from $Z = 11$ to 20 to the extent of the first-order approximation are calculated using the energies and wave functions obtained from the FCPC method. The close agreement among the f-values obtained from the length, velocity, and acceleration formulas indicates that the wave functions are accurate in the whole configuration space, and the f-values obtained in this paper are in satisfactory agreement with experimental data available in the literature. By combining with QDT, the reliable and accurate oscillator strengths for the transitions from the same initial state $1s^2 2s$ to all the final states of the Rydberg series $1s^2 np$, including continuum states, are obtained. We hope our theoretical predictions will provide a valuable reference for experimental measurements and other research in the future.

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References

[1] Kono A and Hattori S 1984 *Phys. Rev.* A **30** 2093
[2] Cann K M and Thakkar A J 1992 *Phys. Rev.* A **46** 5397
[3] Drake G W F 1996 *Atomic, Molecular, and Optical Physics Handbook* (New York: AIP Press) p154
[4] Yan Z C, Tambasco and Drake G W F 1998 *Phys. Rev.* A **57** 1652
[5] Chung K T 1991 *Phys. Rev.* A **44** 5421
[6] Wang Z W and Chung K T 1994 *J. Phys.* B **27** 855
[7] Guan X X and Wang Z W 1998 *Phys. Lett.* **15** 489
[8] Ge Z M, Wang Z W, Zhou Y J, He L M and Liu G G 2003 *Chin. Phys.* **12** 488
[9] Hu M H and Wang Z W 2004 *Chin. Phys.* **13** 662
[10] Hu M H and Wang Z W 2004 *Chin. Phys.* **13** 1246
[11] Hu M H and Wang Z W 2005 *Chin. Phys. Lett.* **22** 1089
[12] Chen C and Wang Z W 2005 *Commun. Theor. Phys.* **43** 305
[13] Wang Z W, Yang D, Hu M H, Han Q J and Li J Y 2005 *Chin. Phys.* **14** 1559
[14] Hu M H and Wang Z W 2008 *Chin. Phys.* B **17** 908
[15] Wang Z W, Liu Y, Hu M H, Li X R and Wang Y N 2008 *Chin. Phys.* B **17** 2909
[16] Wang Z W, Wang Y N, Hu M H, Li X R and Liu Y 2008 *Sci. Chin.* G **51** 1633
[17] Weiss A W 1963 *Astrophys. J.* **138** 1262
[18] Cowan R D 1981 *The Theory of Atomic Structure and Spectra* (Berkeley, CA: University of California Press) p401
[19] Friedrich H 1991 *Theoretical Atomic Physics* (Berlin: Springer) p117
[20] Kim Y S and Praat Y H 1981 *Phys. Rev.* A **24** 1626
[21] Zilitis V A 1984 *Opt. Spec.* **55** 127
[22] Martin G.A and Wiese W L 1976 *J. Chem. Ref. Data* **5** 537