Theoretical study on $2s2p^6np$ Rydberg states of Cu^{19+} ion*

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We report on the calculations of transition wavelengths and weighted oscillator strengths for $2s^22p^6$–$2s2p^6np$ ($4 \le n \le 20$) electric dipole (E1) transitions of Cu^{19+} ion. The flexible atomic code (FAC) has been adopted for the calculations. Comparisons are made with the experimental data available, showing that the present results for $4 \le n \le 6$ are more accurate than the previous calculated values. Furthermore, combining the quantum defect theory (QDT) with the transition energies of $2s^22p^6$–$2s2p^6np$, the quantum defects for $2s2p^6np$ Rydberg series of Cu^{19+} ion are determined. In addition, the energies of any highly excited states ($n > 20$) for this series can be reliably predicted using the QDT and the given quantum defects. The ionization energies for Cu^{19+} and Cu^{20+} ions are also calculated and they excellently accord with previous experimental and calculated values.

Keywords: Cu^{19+}ion, transition wavelength, quantum defect, quantum defect theory

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1. Introduction

Accurate calculations of the Rydberg series of highly charged ions are important for three main reasons. Firstly, accurate calculations of transition wavelengths can achieve rigorous line identification of the observed spectra in experimental surveys and X-ray astrophysics. Secondly, such calculations are conducive to the development of spectroscopic methods for high-temperature plasma diagnosis. Finally, the calculations of a sufficient number of transitions along the Rydberg series allow the accurate determination of ionization energies.

Over the last decade, many integrated packages have been employed to calculate various atomic processes and rich calculations have been generated on generating atomic data (such as energy levels, radiative rates, oscillator strengths, collision strengths and excitation rates) for Fe, Ti, Au, Cr and Ni ions.[1−12] However, theoretical studies on Cu ions, particularly the highly excited Cu ions, are relatively scarce to date. In addition, recent astronomical research [13,14] has shown that the optical lines of the copper ion are important for calculating the abundance of copper for dwarf stars. Therefore, atomic data for Cu^{19+} (including other highly charged copper ions) may be useful for diagnosing a variety of plasmas, such as astrophysical, fusion and laser generated plasmas. For this purpose, we calculate the transition wavelengths and oscillator strengths for $2s^22p^6$–$2s2p^6np$ ($4 \le n \le 20$) of Ne-like Cu^{19+} ions in the present work. The quantum defects for $2s2p^6np$ Rydberg series of this ion are also determined by combining the quantum defect theory (QDT) with the transition energies of $2s^22p^6$–$2s2p^6np$. Based on the above calculations, the theoretical prediction on the energies of this series is accurately extrapolated to the whole energy region of Cu^{19+} ion. For our calculations of transition wavelengths and oscillator strengths, we adopt a fully relativistic configuration-interaction code, i.e. flexible atomic code (FAC),[15−17] in which the atomic structure calculation is based on the relativistic configuration interaction (CI) with independent particle basis wavefunctions. These basis wavefunctions are derived from a local central potential, which is self-consistently determined to represent electronic screening of the nuclear potential. Relativistic effects are fully taken into account through using the

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Dirac-Coulomb Hamiltonian. Higher order quantum electrodynamics (QED) effects are included through Breit interaction in the zero energy limit for the exchanged photon, and hydrogenic approximations for self-energy and vacuum polarization effects.

2. Transition wavelengths and oscillator strengths

There are two series of transitions that arise from $2s^22p^6$–$2s2p^6np$ excitations. The wavelengths of these transitions are in the hard X-ray region. This is one of the important properties of highly ionized atomic systems, which differs from those of neutral atoms or lowly ionized atoms.[18] In the present work, we use the standard notation for Cu^{19+} ion transitions in Ref. [11]: nA: 2s-$np_{3/2}$, nB: 2s-$np_{1/2}$. Furthermore, it is worth noting that the levels of $2s2p^6(n+1)l$ and $2s^22p^5(n+2)l$ configurations are considered in the present work, which have a close interaction with the levels of the $2s2p^6np$ series.

The calculated results of wavelength $\lambda_{\rm FAC}$ for these transitions ($4 \le n \le 6$) of Cu^{19+} ion are listed in Table 1. Also included in the table are the data of experiment and theoretical calculations ($\lambda_{\rm RELAC}$) of Fournier *et al.*,[10–12] who adopted the RELAC code,[19,20] and the spectral resolution is better than $\lambda/\Delta\lambda = 3000$ in their experiment. As listed in Table 1, for the 4A (8.3859 Å) and 4B (8.3998 Å) transitions, the calculated wavelengths are ∼8 mÅ longer than the observed ones; for the 5A (7.6822 Å) transition, the agreement is better, ∼1 mÅ; and for the 6A (7.3462 Å) transition, the calculated wavelength is ∼7 mÅ longer than the observed one. Furthermore, our results are in excellent agreement with the experimental data and better than the values of RELAC, which show that our calculation is reliable. On this basis, the detailed predictions of the wavelengths for $2s^22p^6$–$2s2p^6np$ ($7 \le n \le 20$) transitions are obtained for the first time and listed in Table 2. Table 2 shows that the difference between the wavelengths of nA and nB reduces with the increase of the principal quantum number n, which is 1.8 mÅ for $n = 7$ and ∼ 0.07 mÅ for $n = 20$. Although no experimental data are available for comparison, we believe that the prediction for these transitions is accurate.

Table 1. Calculated transition wavelengths for high-n series members in Ne-like Cu^{19+} ions ($4 \le n \le 6$).

Label	Experiment[10]	Theory			
		This work		RELAC[10–12]	
		$\lambda_{\rm FAC}$/Å	$\Delta\lambda_1$/Å	$\lambda_{\rm RELAC}$/Å	$\Delta\lambda_2$/Å
4A	8.3859	8.3936	–7.7[–3]	8.3684	1.75[–2]
4B	8.3998	8.4077	–7.9[–3]	8.3820	1.78[–2]
5A	7.6822	7.6834	–1.2[–3]	7.6612	2.10[–2]
5B		7.6892		7.6669	
6A	7.3462	7.3530	–6.8[–3]	7.3319	1.43[–2]
6B		7.3561			

$x[y] = x \times 10^y$

Table 2. Calculated transition wavelengths for high-n series members in Ne-like Cu^{19+} ions ($7 \le n \le 20$).

Label	$\lambda_{\rm FAC}$/Å	Label	$\lambda_{\rm FAC}$/Å
7A	7.1698	14A	6.8241
7B	7.1716	14B	6.8243
8A	7.0568	15A	6.81028
8B	7.0580	15B	6.81043
9A	6.9820	16A	6.79902
9B	6.9828	16B	6.79915
10A	6.9297	17A	6.78974
10B	6.9303	17B	6.78985
11A	6.8918	18A	6.7820
11B	6.8922	18B	6.78209
12A	6.8633	19A	6.77546
12B	6.8636	19B	6.77554
13A	6.8414	20A	6.7699
13B	6.8416	20B	6.76997

The calculated weighted oscillator strengths gf (g is the statistical weight of the initial state of a transition, and f is the oscillator strength for the transition) for $2s^22p^6$–$2s2p^6np$ ($4 \le n \le 20$) of Cu^{19+} ion are listed in Tables 3 and 4, and summarized in Fig. 1 along with the available results of Fournier *et al.*[10] As listed in Table 3, the present gf-values accord well with those of Fournier *et al.* within 10% for $4 \le n \le 6$. Additionally, Fig. 1 and Tables 3 and 4 show that the gf-values follow an n^{-3} fall off and rapidly decreases with the increase of principal quantum number in a range of $4 \le n \le 11$, while when $n > 11$, they keep almost unchanging (the relative variations are only 10^{-3} and 10^{-4} for nA and nB, respectively).

Table 3. Weighted oscillator strengths gf for $2s^22p^6$–$2s2p^6np$ of Cu^{19+} ion ($4 \le n \le 6$).

Label	gf[a)]	gf[b)]	Label	gf[a)]	gf[b)]
4A	1.253[-1]	9.682[-2]	5B	1.117[-2]	1.031[-2]
4B	2.529[-2]	3.350[-2]	6A	2.786[-2]	2.597[-2]
5A	5.314[-2]	5.031[-2]	6B	5.975[-3]	

$x[y] = x \times 10^y$

a) results of the present work, b) results of Ref. [10].

Table 4. Weighted oscillator strengths gf for $2s^22p^6$–$2s2p^6np$ of Cu^{19+} ion ($7 \le n \le 20$).

Label	gf	Label	gf
7A	1.654[–2]	14A	1.819[–3]
7B	3.586[–3]	14B	4.034[–4]
8A	1.066[–2]	15A	1.470[–3]
8B	2.327[–3]	15B	3.263[–4]
9A	7.288[–3]	16A	1.205[–3]
9B	1.599[–3]	16B	2.677[–4]
10A	5.210[–3]	17A	1.000[–3]
10B	1.147[–3]	17B	2.224[–4]
11A	3.857[–3]	18A	8.395[–4]
11B	8.510[–4]	18B	1.867[–4]
12A	2.936[–3]	19A	7.116[–4]
12B	6.492[–4]	19B	1.583[–4]
13A	2.288[–3]	20A	6.083[–4]
13B	5.069[–4]	20B	1.354[–4]

$x[y] = x \times 10^y$

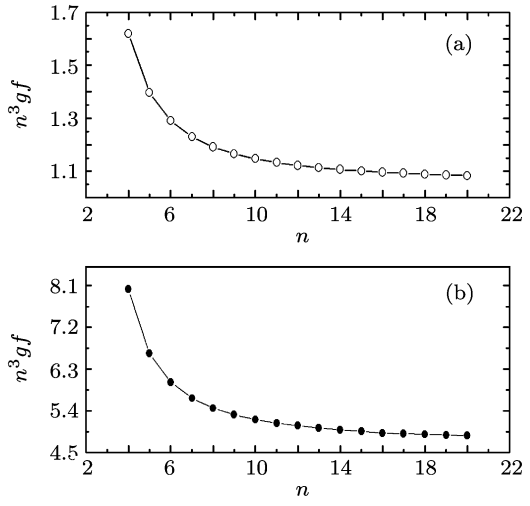


Fig. 1. The gf values for the nA and nB transitions multiplied by n^3: (a) nB, (b) nA.

3. Quantum defects

According to QDT,[21,22] the quantum defect μ_n is defined as (in a.u.)

$$E_n = -\frac{Z_c^2}{2\left(n-\mu_n\right)^2}, \qquad (1)$$

where $Z_c = Z - N + 1$ (Z is the nuclear charge and N is the number of electrons in system), n is the principal quantum number, and E_n is the term energy, which can be obtained from FAC. By using Eq. (1) and the transition energies corresponding to the wavelengths in Tables 1 and 2, the quantum defects $\mu_{n,3/2}$ and $\mu_{n,1/2}$ are calculated, respectively for $2s2p^6np_{3/2}$ and $2s2p^6np_{1/2}$ ($4 \le n \le 20$) Rydberg series of Cu^{19+} ion. The results along with the difference between them ($\Delta\mu_n = \mu_{n,3/2} - \mu_{n,1/2}$) are listed in Table 5 and illustrated in Fig. 2. As shown in Fig. 2, both $\mu_{n,3/2}$ and $\mu_{n,1/2}$ reduce about 0.011 with the principal quantum number n increasing from 4 to 11, while when $n > 11$, they almost keep unchanging, which is about 0.2844 for both $\mu_{n,3/2}$ and $\mu_{n,1/2}$. Therefore, one can calculate the energy of any of the highly excited states ($n > 20$) for this series of Cu^{19+} using Eq. (1) and the quantum defect. In addition, that $\mu_{n,3/2}$ is always bigger than $\mu_{n,1/2}$ for a given n shows the normal fine structure of this Rydberg series of Cu^{19+} ions.[23] Furthermore, $\Delta\mu_n$ also decreases with n increasing in a range of $4 \le n \le 20$ and it follows a well-behaved variation regularity of spin-orbit interaction with n along a Rydberg series, which is the main physical reason resulting in the fine structure of the term energy.[18]

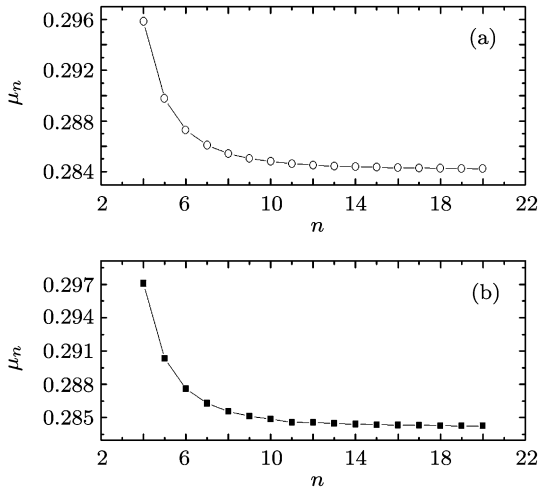


Fig. 2. Values of quantum defect μ_n for $2s2p^6np$ Rydberg series of Cu^{19+}ion: (a) $\mu_{n,1/2}$, (b) $\mu_{n,3/2}$.

Table 5. Quantum defects for $2s2p^6np$ Rydberg series of Cu^{19+} ion.

n	$\mu_{n,3/2}$	$\mu_{n,1/2}$	$\Delta\mu_n$	n	$\mu_{n,3/2}$	$\mu_{n,1/2}$	$\Delta\mu_n$
4	0.297088	0.295842	0.001246	13	0.284477	0.284448	0.000029
5	0.290352	0.289770	0.000582	14	0.284414	0.284390	0.000024
6	0.287610	0.287281	0.000329	15	0.284367	0.284347	0.000020
7	0.286287	0.286085	0.000202	16	0.284330	0.284315	0.000015
8	0.285565	0.285432	0.000133	17	0.284303	0.284289	0.000014
9	0.285137	0.285044	0.000093	18	0.284280	0.284269	0.000011
10	0.284866	0.284800	0.000066	19	0.284263	0.284254	0.000009
11	0.284569	0.284638	0.000069	20	0.284249	0.284241	0.000008
12	0.284565	0.284527	0.000038				

Table 6. Summary of ionization energies (in eV) of Cu^{19+} and Cu^{20+}.

Measured I_{19}	Calculated I_{19}	Measured I_{20}	Calculated I_{20}	Measured δI
1689.30 ± 2.5[a)]	1689.67[b)]	1708.62 ± 2.5[a)]	1710.57[b)]	19.32[a)]
	1690[c)]			20.93±0.01[e)]
	1697[d)]			
	1687.22[f)]		1708.09[f)]	20.87[f)]

a) Ref. [25], b) Ref.[10]–[12], c) Ref. [26], d) Ref. [27], e) Ref. [24], f) Results of the present work.

By fitting the quantum defects and energies obtained above for $2s2p^6np$ ($4 \le n \le 20$) Rydberg series of Cu^{19+} ion, the polynomial functions of μ_n versus E_n are obtained as (in a.u.)

$$\mu_{n,3/2} = -0.0001E_{n,3/2}^2 + 0.0053E_{n,3/2} + 0.2784, \quad (2)$$

and

$$\mu_{n,1/2} = -0.0001E_{n,1/2}^2 + 0.0042E_{n,1/2} + 0.2902, \quad (3)$$

where the last terms of Eqs. (2) and (3) are the ionization thresholds, respectively. The values of quantum defect μ_n vary smoothly with the energies for this Rydberg series, which accords with the QDT. It means that the present quantum defects for this series are reliable.

The ionization energies of Cu^{19+} and Cu^{20+} ions are also calculated to be 1687.22 and 1708.09 eV, respectively. The results and some other available data[10−12,24−27] are also summarized in Table 6. Comparison of the present results with the measured value indicates that the relative discrepancies between them are less than 2.1 eV. The difference between the two ionization energies I_{19} and I_{20}, $\delta I = I_{20} - I_{19}$ accord with the experimental value of 20.93 eV given by Hinnov *et al.* in 3‰, and with the measured value of 19.32 eV given by Fournier *et al.* in 7.4%.

4. Conclusion

In the present work, the transition wavelengths and weighted oscillator strengths for $2s^22p^6$–$2s2p^6np$ ($4 \le n \le 6$) E1 transitions of Cu^{19+} ion are calculated by employing FAC. The comparison between the available experimental results and the present results shows that the present results are more accurate than those from RELAC. The theoretical predictions of transition wavelengths and weighted oscillator strengths for these transitions are also given for $7 \le n \le 20$. Additionally, the values of quantum defect μ_n for $2s2p^6np$ Rydberg series are calculated by combining QDT with the transition energies of $2s^22p^6$–$2s2p^6np$. It is shown that the values of quantum defect μ_n decreases rapidly with the increase of principal quantum number in a range of $4 \le n \le 11$, while keeps nearly unchanging when $n > 11$. On this basis, one can compute the energy of any of the highly excited states ($n > 20$) for this series of Cu^{19+} using the QDT and the given quantum defect. Finally, the polynomial functions of μ_n versus E_n are obtained for this series by fitting the calculated quantum defects and energies. The ionization energies of Cu^{19+} and Cu^{20+} ions are also calculated and in good agreement with the correlative experimental values.

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