Electron-impact study in the valence and autoionization resonance regions of neon

Z. P. Zhong, S. L. Wu, R. F. Feng, B. X. Yang, Q. Ji, and K. Z. Xu
Department of Modern Physics, University of Science and Technology of China, Hefei, Anhui 230027, People's Republic of China

Y. Zou
Institute of Applied Physics and Computational Mathematics, Beijing 100080, People's Republic of China

Jia-Ming Li
Institute of Physics, Chinese Academy of Science, Beijing 100080, People's Republic of China
(Received 6 May 1996)

The recently built electron-energy-loss spectrometer (EELS) (typical full width at half maximum of 60 meV) has been employed to measure EELS spectra of neon in discrete and autoionization resonance regions at a 2.5 keV impact energy and a mean scattering angle of 0°. Relative optical oscillator strength density spectra were established by multiplying the EELS spectra by the known Bethe-Born conversion factor of the spectrometer, and then were normalized at a single point in the smooth continuum. Absolute optical oscillator strengths corresponding to these energy regions are reported and compared with previously published experimental and theoretical values. Two forbidden transitions in the autoionization region are observed and identified. One of them has not been previously reported to our knowledge. [S1050-2947(97)03502-6]

PACS number(s): 32.70.Cs, 32.80.Dz, 34.80.Dp

I. INTRODUCTION

The investigation of optical oscillator strengths (OOSs) and energy levels for neon in discrete and continuum electronic excitation regions is of practical use in providing information for such areas as plasma physics, biophysics, and astronomy. In addition, the study of the electronic excitation of neon is required for evaluation of theoretical atomic-structure calculations.

For the excitation of neon in discrete and autoionization resonance regions, previous works in these regions have been quoted in detail by Chan *et al.* [1]. Briefly, for the discrete region, experimental methods avoiding the line-saturation effect, which may result in serious errors in measurements for the extremely narrow valence-shell electronic transitions [2], have employed such techniques as profile analysis [3,4], self-absorption [5–7], total absorption [8], lifetime measurements [9–16], and electron-impact based methods [1,17–20]. Theoretical calculations have been reported by a number of authors [8,11,21–31] using various methods. However, most of these measurements and calculations gave only the absolute optical oscillator strength values for the $2s^2 2p^5(2P_{3/2})3s$ and $2s^2 2p^5(2P_{1/2})3s'$ excitations, some of them gave more OOS values, but these values show a considerable spread for some states. Some experimental groups [1,8,32,33] have studied, in some detail, the autoionizing resonance region of neon.

In this paper, the absolute optical oscillator strength values for electronic transitions corresponding to the regions 15.8–22.2 eV and 43.0–55.0 eV are reported using a highly accurate dipole (e,e) electron-energy-loss spectrometer (EELS) method which was applied to an electron-impact study in the valence and autoionization resonance regions of argon [34]. Using the spectrometer at the same experimental conditions, excellent agreement was found between our work and Chan *et al.* [35] using the same method for the measured regions of argon. In this work, these results are compared with previously published experimental and theoretical values. Two forbidden transitions in the autoionization resonance region are observed and denoted.

II. EXPERIMENTAL METHOD

The apparatus employed in this work is a recently built high-resolution double hemispherical electron-energy-loss spectrometer. Details of the apparatus were described in our previous works [34,36]. Briefly, it consists of an electron gun, a hemispherical electrostatic monochromator, a rotatable energy analyzer, of the same type, and an interaction chamber. All of these components are enclosed in four individual vacuum chambers. The impact energy can be varied from 1.0 keV to 5.0 keV. The instrumental typical energy resolution was 60 meV full width at half maximum (FWHM). The measurements were at a 2.5 keV impact energy and a mean scattering angle of 0°, with an acceptance angle of 2.0×10^{-4} sr. The measured spectra were the sum of many repetitive scans. The background pressure in the vacuum chambers was 3.0×10^{-5} Pa. Relative optical oscillator strength density spectra were obtained by multiplying the electron-energy-loss spectra by the known Bethe-Born conversion factor of the spectrometer. The used method was referred to in Ref. [2] and determined in Ref. [36]. Absolute scales were obtained by normalizing at a single point in the smooth continuum using absolute values recently reported by Chan *et al.* [1].

Since background gases remained at the base pressure, these contributions were removed by subtracting the signal when the pressure of neon was one-fifth of the gas sample pressure in all the above measurements. Energy scales of the spectra were calibrated using the discrete excitation transition $2s^2 2p^6 \rightarrow 2s^2 2p^5(2P_{1/2})3s'$ which occurred at 16.848 eV [37].

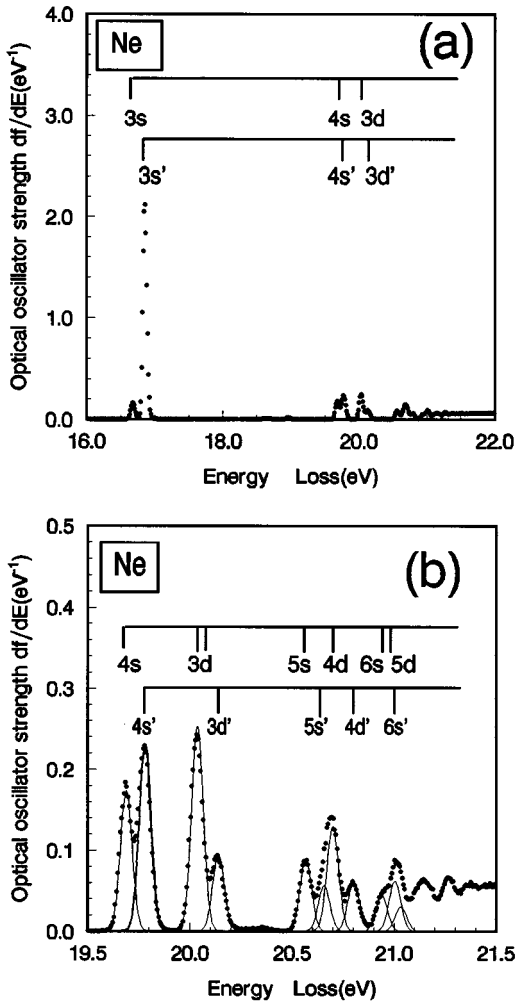

FIG. 1. Absolute optical oscillator strength density spectrum of neon in the discrete region. (a) 15.7–22.2 eV at energy-loss steps of 12.5 meV. (b) Expanded view of the 19.0–21.6 eV energy region with 6.25 meV steps. The deconvoluted peaks are plotted as solid lines.

III. RESULTS AND DISCUSSIONS

A. Absolute optical oscillator strengths in valence excitation region

Figure 1(a) shows resulting spectra of neon in the discrete region 15.8–22.2 eV normalized at 22.0 eV. The energy-loss interval is in 12.5 meV steps. The assignments of the various members of the nl and nl' series indicated in Fig. 1 are taken from Ref. [37]. The completely resolved peaks, the $3s$ and $3s'$ resonance lines, were integrated from the respective peak areas to determine absolute optical oscillator strengths. For the partially resolved or unresolved peaks at higher energies, a least-square curve fitting program was used to deconvolute these peaks and determine the absolute optical oscillator strength of respective peak. Because these transitions have extremely narrow natural linewidths, neglecting the influence of natural line profiles of discrete electronic transitions of neon is reasonable. The experimental line profile is well described by the instrumental function which can be described by the weighted sum of a 96% Gaussian profile and a 4% Lorentzian profile. Fig. 1(b) shows an expanded view of the deconvoluted peaks and the absolute optical oscillator strength density spectrum in the 19.0–21.6 eV energy region in 6.25 meV steps. Since the energies of peaks for the $nd[1/2]$ and $nd[3/2]$ states which converge to the same $^2P_{3/2}$ limit are very close, especially at higher n values, the two transitions have been treated as a single peak in the deconvolution.

The resulting values obtained from analysis of the spectra are shown in Table I. The experimental errors in this work mainly result from these factors: the errors resulted from the Bethe-Born factor conversion of the instrument, the statistical uncertainties, the uncertainties in making data absolute, the double scattering, and the uncertainties of gas pressure. Moreover, the errors of the deconvolution procedure should be considered for the partially resolved or unresolved peaks. The estimated errors in the experimental measurements are listed in parentheses in Table I. Because the previous works of neon in the discrete region have been tabulated by Chan *et al.* [1], results from major groups are listed in Table I. Clearly, our results are generally in satisfactory agreement with the values determined by Chan *et al.* [1] for all transitions in Table I. The electron-impact results obtained by Natali, Kuyatt, and Mielczarek [19], quoted in Ref. [6], are most consistent with the present work, while for some states discrepancies are up to 38%. The data of Suzuki *et al* [20] on the optical oscillator strengths of $2s^2 2p^5(2P_{3/2})3s$ and $2s^2 2p^5(2P_{1/2})3s'$ states obtained by extrapolating generalized oscillator strengths to zero momentum transfer are lower than this work and are consistent within experimental errors. For the optical methods, the data using the self-absorption method performed by Westerveld, Mulder, and Van Eck [6] are mostly lower than this work by 4%–12%, but still within the quoted uncertainties. While the data of Aleksandrov *et al.* [8] employing the total absorption method show generally higher values by 10%–45%, however for the state $3s$ and $3s'$, their data are lower than our results. The data of Lawrence and Liszt [10], obtained by lifetime measurement, show lower values except that the data of $3d'$ and $5s$ states are in good agreement with our work. Theoretically, the values obtained by Aleksandrov *et al.* [8] using an intermediate-coupling scheme are generally consistent with our results, while they show lower results for $3s$ and $3s'$ states. The summed optical oscillator strengths reported by Cooper [22] and Kelly [23] are in agreement with this work within the experimental errors.

B. Absolute optical oscillator strengths in inner valence-excitation region

The energy region in 43.0–54.0 eV is the autoionization resonance region of neon involving the excitation of inner valence $2s$ electrons and the double excitation of $2p$ electrons. The resulting optical oscillator strength density spectra, which were normalized at a single point in the smooth continuum at 43.0 eV, are shown in Fig. 2(a) (in 10 meV energy steps) and Fig. 2(b) (in 21.48 meV steps). It should be mentioned that detailed high-resolution absolute intensity measurements have been published for neon in these regions only by this work and Chan *et al.* [1] to the best of our knowledge. The resolution in our measurement is typically 60 meV FWHM, however it is 98 meV FWHM for Chan

TABLE I. Experimental and theoretical absolute optical oscillator strength values of neon in discrete region (estimated errors in experimental measurements are listed in parentheses).

	Oscillator strength for transition from $2s^2 2p^6 \rightarrow 2s^2 2p^5 m$ where m is					
	$(^2P_{3/2})3s$	$(^2P_{1/2})3s'$	$(^2P_{3/2})4s$	$(^2P_{1/2})4s'$	$(^2P_{3/2})3d$	$(^2P_{1/2})3d'$
Experimental						
(1) electron-impact method						
the present work	0.0124	0.156	0.0126	0.0167	0.0183	0.006 87
	(0.0038)	(0.009)	(0.0006)	(0.0007)	(0.0008)	(0.000 32)
Ref. [1]	0.0118	0.159	0.0129	0.0165	0.0186	0.006 65
	(0.0006)	(0.008)	(0.0006)	(0.0008)	(0.0009)	(0.000 33)
Ref. [19]	0.012	0.158	0.013	0.016	0.017	0.006
Ref. [20]	0.0106	0.137				
	(0.0014)	(0.018)				
(2) optical methods						
Ref. [8] (total absorption)	0.012	0.144	0.0145	0.0185	0.0222	0.0082
	(0.003)	(0.024)	(0.0035)	(0.006)	(0.0046)	(0.0029)
Ref. [6] (absolute self-absorption)	0.0109	0.147	0.0128	0.0153		0.0064
	(0.0008)	(0.012)	(0.0010)	(0.0012)		(0.0005)
Ref. [10] (lifetime)	0.0078	0.130	0.0086	0.0130	0.0217	0.0064
	(0.0004)	(0.013)	(0.0010)	(0.0020)	(0.0022)	(0.0010)
Theoretical						
Ref. [8]	0.0106	0.141	0.0124	0.0160	0.0176	0.0064
Ref. [22][a]	0.163		0.026		0.037	
Ref. [23][a]	0.188		0.029		0.036	

	Oscillator strength for transition from $2s^2 2p^6 \rightarrow 2s^2 2p^5 m$ where m is						
	$(^2P_{3/2})5s$	$(^2P_{1/2})5s'$	$(^2P_{3/2})4d$	$(^2P_{1/2})4d'$	$(^2P_{3/2})6s$	$(^2P_{1/2})6s'$	$(^2P_{3/2})5d'$
Experimental							
(1) electron-impact method							
the present work	0.006 45	0.004 07	0.009 37	0.004 47	0.003 24	0.002 20	0.004 49
	(0.000 18)	(0.0029)	(0.000 37)	(0.000 13)	(0.000 19)	(0.000 45)	(0.000 52)
Ref. [1]	0.006 37	0.004 61	0.009 44	0.004 39	0.003 30	0.001 56	0.005 43
	(0.000 32)	(0.000 23)	(0.000 32)	(0.000 22)	(0.000 30)	(0.000 16)	(0.000 54)
Ref. [19]	0.006	0.0043	0.0085	0.0043			
(2) optical methods							
Ref. [8] (total absorption)	0.0083	0.0049	0.0147	0.005	0.0045	0.003	
	(0.0031)	(0.0017)	(0.0036)	(0.002)	(0.0019)	(0.001)	
Ref. [6] (absolute self-absorption)	0.0061	0.0042					
	(0.0005)	(0.0003)					
Ref. [10] (lifetime)	0.0057	0.0042					
	(0.0010)	(0.0010)					
Theoretical							
Ref. [8]	0.0060	0.0043	0.0091	0.0041	0.0031	0.0018	0.0050
Ref. [22][a]	0.009		0.020		0.004		
Ref. [23][a]	0.008		0.025		0.003		

[a]Summed oscillator strength as indicated.

et al. [1]. Similar to the situation for electron-energy-loss spectra in the valence-shell excitation transition region, the present work shows good agreement with the work of Chan *et al.* [1] in the terms of both shape and absolute values. The absolute values measured by Samson [38,39] are reasonably consistent with the present work.

The energies of the transitions corresponding to excitation of the $2s$ electron to np subshell ($n=3$–6), and the double excitation of two $2p$ electrons to the $3s3p$ configuration of neon have been listed in Table II, the error of each energy value in this work is 10 meV. Two very small peaks at 43.717 eV and 46.639 eV can be observed in the present work. The peak at 43.736 eV is also reported by Chan *et al.* [1], Simpson, Chamberlain, and Mielczarek [40] using a lower electron-impact energy ($\leqslant$400 eV), and Brion and Olsen [42] with a threshold electron-impact study. Simpson,

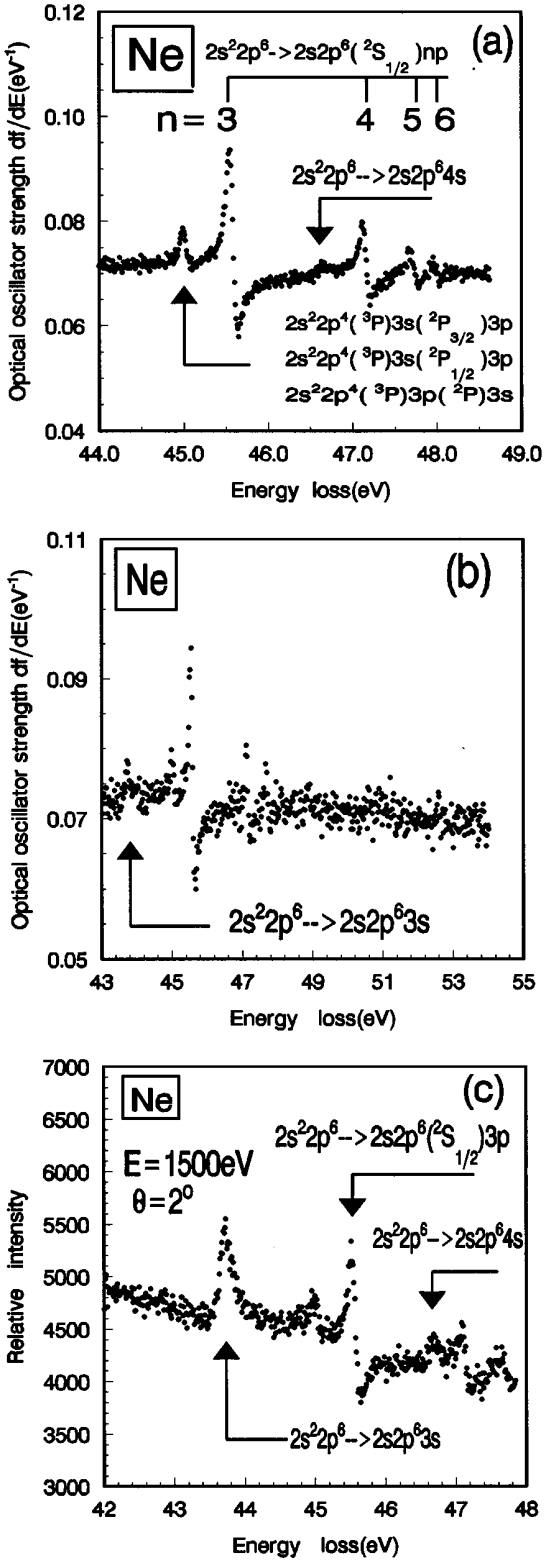

FIG. 2. (a) Absolute optical oscillator strength density spectrum of neon in the autoionizing resonance region of 44.0–48.6 eV in energy-loss steps of 10 meV. (b) Absolute optical oscillator strength density spectrum of neon in the autoionizing region of 43.0–54.0 eV in energy-loss steps of 21 meV. (c) The electron-energy-loss spectrum of neon in the 42.0–47.8 eV region obtained at 1.5 keV impact energy (100 meV FWHM) and a mean scattering angle of 2.0°. The states of interest are $2s2p^6 3s$ at 43.717 eV, $2s2p^6 4s$ at 46.639 eV.

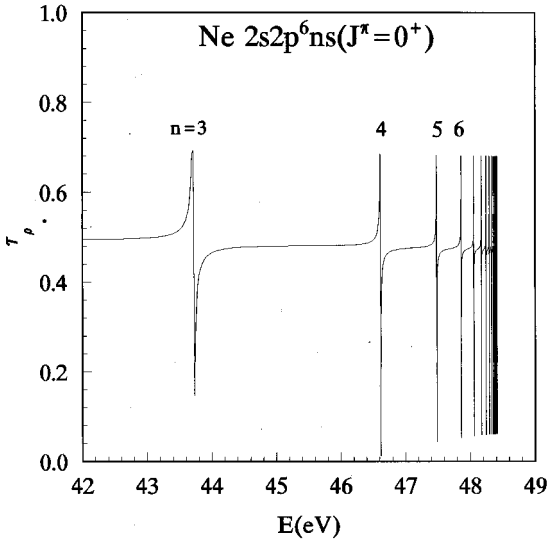

FIG. 3. Collision eigenphase shifts $\pi\tau_\rho$ for the $2s2p^6 ns(J^\pi = 0+)$ resonances.

Chamberlain, and Mielczarek [40], and Brion and Olsen [42] suggested that this was probably a contribution from the dipole-forbidden state $2s2p^6 3s$. Siegbahn *et al.* [41] have reported that the energy of $2s2p^6 3s$ level is 43.65 eV. However, Chan *et al.* [1] thought that the formally dipole-forbidden transition $2s^2 2p^6 \rightarrow 2s2p^6 3s$ would not be so prominent at the very low-momentum transfer (0.014 a.u.) under their experimental conditions. Our previous work on argon [34] at the present experimental conditions has showed that optically forbidden transition can be detected even when the momentum transfer is smaller than 0.01 a.u. To go further into the question, we measured the electron-energy-loss spectrum at a 1.5 keV impact energy (100 meV FWHM) and a mean scattering angle of 2.0° in the energy region 42.0–48.0 eV, which is shown in Fig. 2(c). By comparing Fig. 2(b) with Fig. 2(c), it is obvious that the ratio of areas for the peak at 43.717 eV, to the peak corresponding to the optically allowed transition at 45.543 eV is much higher as the momentum transfer increases. The same is also true for the ratio of areas for the peak at 46.639 eV to the peak corresponding to the optically allowed transition at 47.119 eV. So it may be concluded that the peaks at 43.717 eV and 46.639 eV come from optically forbidden transition. The peak at 46.639 eV is reported for the first time, to our knowledge. We calculated some energy levels of optically forbidden transitions and optically allowed transitions for neon in the above energy region by our recently developed relativistic multichannel theory [43,44]. Figure 3 displays collision eigenphase shifts $\pi\tau_\rho$ for the $2s2p^6 ns(J^\pi = 0^+)$ resonance states. The calculated energies and other groups' energies are also listed in Table II. Clearly, our theoretical energies of optically allowed transitions are in agreement with the high-resolution experimental studies reported by this experimental work, Chan *et al.* [1], Codling, Madden, and Ederer [32], and Aleksandrov *et al.* [8], as well as with the multiconfiguration close-coupling calculations of Luke [45]. Therefore, we may identify the two unknown peaks as $2s2p^6 3s$ and $2s2p^6 4s$.

TABLE II. Experimental and theoretical energy levels for neon (energies in eV).

	Energy levels for transition from $2s^2 2p^6 \rightarrow$						
	$2s2p^6 3s$	$2s^2 2p^4 3s3p$	$2s2p^6 3p$	$2s2p^6 4s$	$2s2p^6 4p$	$2s2p^6 5p$	$2s2p^6 6p$
Experimental							
This work	43.717	44.984	45.543	46.639	47.119	47.680	47.971
Ref. [1]	43.735	44.999	45.550		47.127	47.677	47.977
Ref. [32]		45.072	45.546		47.121	47.692	47.979
Ref. [8]		45.079	45.642		47.221	47.784	48.061
Ref. [40]	43.7		45.6				
Ref. [42]	43.7						
Theoretical							
This work	43.717		45.417	46.613	47.086	47.680	47.960
Ref. [45]			45.631		47.150	47.707	47.973
Ref. [41]	43.65						

IV. CONCLUSION

Absolute optical oscillator strength data of neon in both discrete and autoionizing resonance regions have been reported using a recently built dipole (e,e) spectrometer at an impact energy of 2.5 keV (typical FWHM is 60 meV) and a mean scattering angle of $0°$. The electron-energy-loss spectra were transformed into the absolute oscillator strength density spectra by multiplying by the Bethe-Born conversion factor of the spectrometer and normalizing at a single point in the smooth continuum region. In the discrete region, the presently reported results were compared with theoretical calculations and experimental data. Absolute optical oscillator strengths for the autoionization resonance region involving inner-valence $2s$ electrons excitation and the double excitation of $2p$ electrons have also been determined. The optical oscillator strength density spectra in these regions are generally in good agreement with the electron-impact based data of Chan *et al.* [1]. Moreover, we have studied optically forbidden transitions in the autonization region in some detail and observed the forbidden transition $2s2p^6 4s$ for the first time, to our knowledge.

[1] W. F. Chan, G. Cooper, X. Guo, and C. E. Brion, Phys. Rev. A **46**, 149 (1992).
[2] W. F. Chan, G. Cooper, and C. E. Brion, Phys. Rev. A **44**, 186 (1991).
[3] F. A. Korolev, V. I. Odintsov, and E. V. Fursova, Opt. Spektrosk. **16**, 555 (1964) [Opt. Spectrosc. (USSR) **16**, 304 (1964)].
[4] E. L. Lewis, Proc. Soc. **92**, 817 (1967).
[5] J. P. De. Jongh and J. Van Eck, Physica **51**, 104 (1971).
[6] W. B. Westerveld, Th. F. A. Mulder, and J. Van Eck, J. Quant. Spectrosc. Radiat. Transfer **21**, 533 (1979).
[7] S. Tsurubuchi, K. Watanable, and T. Arikawa, J. Phys. Soc. Jpn. **59** , 497 (1990).
[8] Y. M. Aleksandrov, P. F. Gruzdev, M. G. Kozlov, A. V. Loginov, V. N. Makhov, R. V. Fedorchuk, and M. N. Yakimenko, Opt. Spektrosk. **54**, 7 (1983) [Opt. Spectrosc. (USSR) **54**, 4 (1983)].
[9] B. Decomps and M. Dumont, IEEE J. Quantum Electron. **QE-4**, 916 (1968).
[10] G. M. Lawrence and H. S. Liszt, Phys. Rev. **178**, 178 (1969).
[11] J. Z. Klose, Phys. Rev. **188**, 45 (1969).
[12] S. Kazantsev and M. Chaika, Opt. Spektrosk. **3**, 510 (1971) [Opt. Spectrosc. (USSR) **3**, 273 (1971)].
[13] D. J. G. Irwin, A. E. Livingston, and J. A. Kernahan, Can. J. Phys. **51**, 1948 (1973).
[14] M. Ducloy, Ann. Phys. (Paris) **8**, 403 (1973).
[15] E. J. Knystautas and R. Drouin, Astron. Astrophys. **37**, 45 (1974).
[16] N. D. Bhaskar and A. Lurio, Phys. Rev. A **13**, 1484 (1976).
[17] J. Geiger, Z. Phys. **177**, 138 (1964).
[18] J. Geiger, Phys. Lett. **33A**, 351 (1970).
[19] S. Natali, C. E. Kuyatt, and S. R. Mielczarek (unpublished).
[20] T. Y. Suzuki, H. Suzuki, S. Ohtani, B. S. Min, T. Takayanagi, and K. Wakiya, Phys. Rev. A **49**, 4578 (1994).
[21] A. Gold and R. S. Knox, Phys. Rev. **113**, 834 (1959).
[22] J. W. Cooper, Phys. Rev. **128**, 681 (1962).
[23] P. S. Kelly, J. Quant. Spectrosc. Radiat. Transfer **4**, 117 (1964).
[24] P. F. Gruzdev, Opt. Spektrosk. **22**, 313 (1967) [Opt. Spectrosc. (USSR) **22**, 170 (1967)].
[25] J. Z. Klose, J. Quant. Spectrosc. Radiat. Transfer **9**, 881 (1969).
[26] M. Aymar, S. Feneuille, and M. Klapisch, Nucl. Instrum. Methods **90**, 137 (1970).
[27] P. F. Gruzdev and A. V. Loginov, Opt. Spektrosk. **35**, 3 (1973) [Opt. Spectrosc. (USSR) **35**, 1 (197)].
[28] R. Albat and N. Gruen, J. Phys. B **7**, L9 (1974).
[29] R. F. Stewart, Mol. Phys. **29**, 1577 (1975).
[30] M. Ya. Amus'ya, *Atomic Photoeffect* (Plenum, New York, 1990), p. 170.
[31] J. A. Simpson, G. E. Chamberlain, and S. R. Mielczarek, Phys. Rev. A **139**, 1039 (1965).
[32] K. Codling, R. P. Madden, and D. L. Ederer, Phys. Rev. **155**, 26 (1967).

[33] A. A. Wills, A. A. Cafolla, A. Svensson, and J. Comer, J. Phys. B **23**, 2013 (1990).
[34] S. L. Wu, Z. P. Zhong, R. F. Feng, S. L. Xing, B. X. Yang, and K. Z. Xu, Phys. Rev. A **51**, 4494 (1995).
[35] W. F. Chan, G. Cooper, X. Guo, G. R. Burton, and C. E. Brion, Phys. Rev. A **46**, 149 (1992); **48** , 858 (1993).
[36] R. F. Feng, B. X. Yang, S. L. Wu, S. L. Xing, F. Zhang, Z. P. Zhong, X. Z. Guo, and K. Z. Xu, Sci. China **39**, 1288 (1996).
[37] C. E. Moore, *Atom Energy Levels*, Natl. Bur. Stand. (U.S.) Circ No. 467 (U.S. GPO, Washington, D.C., 1949), Vol. I, p. 77.
[38] J. A. R. Samson, J. Opt. Soc. Am. **55**, 935 (1965).
[39] J. A. R. Samson, Adv. At. Mol. Phys. **2**, 177 (1966).
[40] J. A. Simpson, G. E. Chamberlain, and S. R. Mielczarek, Phys. Rev. A **139**, 1039 (1965).
[41] K. Siegbahn, C. Nordling, G. Johansson, J. Hedman, P. F. Heden, K. Hamrin, T. Bergmark, L. O. Werme, R. Manne, and Y. Baer, *ESCA: Applied to Free Molecules* (North-Holland, Amsterdam, 1969), p. 152.
[42] C. E. Brion and L. A. R. Olsen, J. Phys. B **3**, 1020 (1970).
[43] Yu Zou, Xiao-Min Tong, Jia-Ming Li, Acta Phys. Sinica **45**, 50 (1995).
[44] Wen Huang, Yu Zou, Xiao-Min Tong, Jia-Ming Li, Phys. Rev. A **52**, 2770 (1995).
[45] T. M. Luke, J. Phys. B **6**, 30 (1973).