Russian Physics Journal, Vol. 39, No. 1, 1996

CALCULATION AND EXTRAPOLATION OF OSCILLATOR STRENGTHS IN Rb-LIKE, MULTIPLY CHARGED IONS

A. V. Glushkov, S. V. Ambrosov, V. É. Orlova, S. V. Orlov, A. K. Balan, N. G. Serbov, and G. M. Dormostuchenko

UDC 539.184

The oscillator strengths of dipole transitions between energy levels of the lowest configurations of ions of the Rb I isoelectronic sequence with nuclear charge Z = 41-46 are calculated on the basis of the model potential method using an energy approach. For certain ions the reported data are published here for the first time. It is shown that the contribution of core polarization to the oscillator strength attains 15% for some transitions.

We have investigated spectroscopic characteristics – the oscillator strengths – of ions of the Rb I isoelectronic sequence. We call attention to the substantial number of papers published on atoms of alkali elements (see, e.g., [1-10]), but only the first terms of the sequence have been studied in detail, mainly for Li-, Na-, and K-like ions. Rubidium-like ions have been investigated to a far lesser degree than, for example, Na- and K-like ions. Data on the energy levels and oscillator strengths for these ions are available mainly for the first terms of the sequence, in particular for Rb I, Sr II, Y III, Zr IV, Nb V, and Mo VI ions, with fairly detailed information for the first three (the values of the oscillator strengths are given for the transitions $nl-n'l'$, $n, n' = 4\text{-}7$; $l, l' = 0\text{-}4$) but minimal information for the other three and then mainly applicable only to certain isolated transitions [9]. One of the most complete studies of Rb-like ions [9] gives data from calculations of the oscillator strengths gf of the above-indicated ions in the nonrelativistic, Coulomb screened potential approximation. We note that the significant role of the core polarization effect, particularly with the transition from a Li atom (for resonance transition, allowance for polarization of the core lowers the value of gf by approximately 1%) to Cs (where the contribution of core polarization to gf for resonance transition is 16%), has been demonstrated previously in the example of calculations for neutral atoms of alkali elements. In the present study we investigate Rb-like ions with nuclear charge $Z = 41\text{-}46$ and calculate the oscillator strengths of the transitions $5s^2S-5p^2P$, $6s^2S-6p^2P$, $5s^2S-6p^2P$, $5p^2P-5d^2D$, and $5p^2P-4d^2D$.

We now discuss briefly the main aspects of calculating the probabilities and oscillator strengths of transitions in the atoms by the energy approach (S-matrix formalism) [10-13]. Within the framework of this approach the probability of radiative decay of an excited atomic state is related to the corresponding imaginary part of the electron energy of the atomic system. In the second perturbation approximation the required imaginary part $\mathrm{Im}\,E$ is given by the expression

$$\mathrm{Im}\,E = -\frac{1}{4\pi}\cdot\sum_{\substack{a>n\\ n>f}} V^{|\omega_{an}|}_{anan}, \tag{1}$$

where the matrix element V is described by an integral of the form

$$V_{ijkl} = \int\int d^3r_1\, d^3r_2\, \psi_i^*(r_1)\,\psi_j^*(r_2)\,\frac{\sin|\omega|r_{12}}{r_{12}}\cdot(1-\alpha_1\alpha_2)\,\psi_k(r_2)\,\psi_l(r_1). \tag{2}$$

The individual terms of the sum over n in Eq. (2) represent the contributions of different channels, the dipole transition probability is

$$\Gamma_{an} = \frac{1}{4\pi}\cdot V^{|\omega_{an}|}_{anan}, \tag{3}$$

Hydrometeorological Institute, Odessa. Translated from Izvestiya Vysshikh Uchebnykh Zavedenii, Fizika, No. 1, pp. 89-92, January, 1996. Original article submitted January 13, 1995.

1064-8887/96/3901-0081$15.00

TABLE 1. Oscillator Strengths of Dipole Transitions in Rb-Like Ions

Ion	Nb V [9]	Mo VI [9]			Tc VII	Ru VIII	Rh IX	Pd X
$5s^2S-5p^2P$	1.12	1.16	1.34	1.35	1.41	1.49	1.56	1.64
$6s^2S-6p^2P$		1.55		1.56	1.58	1.62	1.68	1.73
$5s^2S-6p^2P$		0.31*		0.24*	0.19*	0.16*	0.14*	0.13*
$5p^2P-5d^2D$	1.20	1.22	1.23	1.24	1.27	1.30	1.35	1.38
$5p^2P-4d^2D$	0.106	0.108	0.096	0.098	0.088	0.077	0.069	0.062
$4p^2P-4f^2F$	0.596	0.61	0.679	0.69	0.77	0.85	0.95	1.06

Note: The asterisk denotes (e.g.) $0.31^* = 0.31 \cdot 10^{-3}$.

and the oscillator strength of the corresponding transition is

$$gf = \lambda^2 g' \Gamma_{an} / 6{,}67 \cdot 10^{15}, \tag{4}$$

where g and g' are the degrees of degeneracy, and λ is the wavelength of the transition in angstroms (Å). In the relativistic model potential method, as mentioned in [6, 7], the role of the wave functions is taken by eigenfunctions of the Dirac relativistic Hamiltonian with a model potential $V_c(r)$ that describes the interaction of an outer electron (quasiparticle) with an atomic core of filled electron shells in the given single-quasiparticle atom (ion). Here V_c is interpreted as an Ivanov–Ivanova model potential [8] of the form

$$V_c(r) = -\{Z-2[1-\exp(-2r)(1+r)]-(N-2)[1-\exp(-br)\times \\ \times(1+0{,}75br+0{,}25b^2r^2+0{,}0625b^3r^3)]\}/r. \tag{5}$$

The constants b_κ are evaluated from the known energy levels of the ions. For given energies in the first stage the Dirac equation with the model potential v_c is regarded as an eigenvalue equation in the parameter b. The properly chosen value of b ensures satisfaction of the condition $f(r) \to 0$ and $g(r) \to 0$ in the limits $r \to 0$ and $r \to \infty$ (f and g are the large and small components of the Dirac wave function).

A procedure for determining the matrix elements (2) is set forth, for example, in [11]. The equations given there describe the radiative decay of excited states of an atomic system with one outer electron above a core of filled electron shells. Numerous calculations of transition probabilities and oscillator strengths in atomic systems have shown that it is often very important to take into account the polarization of the core by an outer valence electron (vacancy) in order to achieve accuracy on a par with present-day experimental measurements, particularly in the case of transitions between low-level configurations of atoms and ions [1-10]. A sizable inventory of procedures is currently available for taking this effect into account [8, 15], but the most systematic technique appears to be the quantum-electrodynamical procedure developed in [15]. According to [8, 15], the inclusion of core polarization corresponds to the addition of a secondary polarization potential to the interelectron Coulomb interaction operator in (2) to describe the interaction of an electron with electrodynamic vacuum through a polarizable core. Within the framework of the energy approach this potential is equivalent to the polarization interaction potential of two external particles through the polarizable core in an atomic system with two quasiparticles over a core of filled electron shells. The following expression has been derived [15] for the required potential:

$$V_{pol}(r_1, r_2) = X\{\int dr\, \rho_c^{1/3}(r)\,\Theta(r)/|r_1-r||r-r_2| - \\ -|\int dr \rho_c^{1/3}(r)\,\Theta(r)/|r_1-r|\int dr \rho_c^{1/3}(r)\,\Theta(r)/|r-r_2||/ \\ \int dr \rho_c^{1/3}(r)\,\Theta(r)\}, \quad \Theta(r) = \{1-[3\pi^2\rho_c^{1/3}(r)]/c^2\}^{1/2}$$

(X is a numerical coefficient, ρ_c is the electron density of the core, and c is the speed of light). As noted in [15], the angular parts of the matrix elements of the interelectron Coulomb and polarization interaction operators coincide and, as a result, allowance for polarization of the core merely entails redefining the radial integrals of the radial parts of the matrix elements of the coulomb interaction operator. A computational procedure for determining the required matrix elements is described in detail in [12].

The results of calculations and extrapolation of the oscillator strengths of the indicated transitions for the subject Rb-like ions are summarized in Table 1. Also given in the table are the oscillator strengths of the corresponding transitions, calculated in the screened Coulomb potential approximation [9] for Nb V and Mo VI ions. It is evident form the table that the oscillator strengths calculated in the present study are in good agreement with what appear to be the only other results published to date [9]. To all appearances, the data given for all the other ions are published here for the first time. An analysis of the data demonstrates the critical significance of taking into account the polarization of the core by an outer electron; the inclusion of this effect lowers the values of the oscillator strengths gf by 10-20% for the majority of the transitions. We also note that for Rb-like ions, as in the case of Na-like ions, certain complications can arise not only in setting up an experiment and interpreting its results, but also in comparing the calculated and experimental values of the oscillator strengths (for a more detailed discussion see [14, 16], where this problem is carefully analyzed for ions of the Na I series and for ions of the A II isoelectronic sequence). Nonetheless, our results are of unquestionable interest and can be used in various approximations for the solution of astrophysical problems, the construction of kinetic models of plasma processes, and the investigation of processes in a thermonuclear reactor plasma, whose properties are determined in significant measure by highly ionized impurity atoms, etc.

REFERENCES

1. U. I. Safronova and V. S. Senashenko, Theory of the Spectra of Multiply Charged Ions [in Russian], Nauka, Moscow (1984).
2. I. L. Beigman, L. A. Vainshtein, and V. P. Shevel'ko, Opt. Spektrosk., **28**, No. 3, 425-430 (1970).
3. C. Laughlin and G. A. Victor, Adv. At. Mol. Phys., **25**, 163-194 (1988).
4. J. Migdalek, Can. J. Phys., **54**, No. 1, 130-136 (1976).
5. A. W. Weiss, J. Quant. Spectrosc. Radiat. Transfer, **18**, No. 5, 481-491 (1977).
6. A. V. Glushkov, S. V. Malinovskaya, and V. V. Filatov, Izv. Vyssh. Uchebn. Zaved., Fiz., No. 12, 73-79 (1989).
7. A. V. Glushkov and S. V. Malinovskaya, Izv. Vyssh. Uchebn. Zaved., Fiz., No. 10, 3-9 (1992).
8. L. N. Ivanov and E. P. Ivanova, At. Data Nucl. Data Tables, **24**, No. 2, 95-101 (1979).
9. A. Lingard and S. E. Nielsen, At. Data Nucl. Data Tables, **19**, No. 4, 533-635 (1977).
10. A. V. Glushkov and L. N. Ivanov, Phys. Lett. A, **169**, No. 3, 33-73 (1992).
11. L. N. Ivanov, Abstract of Dissertation for the Degree of Doctor of Physicomathematical Sciences [in Russian], Leningrad (1985).
12. E. P. Ivanova, Author's Abstract of Dissertation for the Degree of Doctor of Physicomathematical Sciences [in Russian], Moscow (1993).
13. M. A. Braun, Yu. Yu. Dmitriev, and L. N. Labzovskii, Zh. Éksp. Teor. Fiz., **57**, No. 6, 2189-2197 (1969) (1970).
14. A. V. Glushkov, S. V. Malinovskaya, and V. V. Filatov, Opt. Spektrosk., **62**, No. 6, 1212-1215 (1987).
15. E. P. Ivanova, L. N. Ivanov, A. V. Glushkov, and A. E. Kramida, Phys. Scr., **32**, No. 4, 512-524 (1985).
16. K. Aashamar, T. Luke, and J. Talman, Phys. Scr., **30**, 121-134 (1984.