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Calculation of Oscillator Strengths for P III, S IV, Cl V, and Ar VI

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We use an analytic potential model adjusted to experimental energy levels to generate wave functions for the valence and excited states of the isoelectronic ions P III, S IV, Cl V, and Ar VI of the aluminum sequence. Using these wave functions in conjuction with the Born approximation and the LS-coupling scheme, we calculate optical oscillator strengths for various excitations of the valence electron. Good agreement is obtained with experimental and theoretical data.

1. INTRODUCTION

Optical oscillator strengths (OOS) are needed in many applications of atomic physics. For example, the OOS can be used to determine various atomic quantities such as the refractive index, the dipole polarizability, and the diamagnetic susceptibility of a system (Stewart, 1967; Dalgarno and Lynn, 1957; Cooper, 1962). In this article we present the results of calculations of OOS for the isoelectronic ions P III, S IV, Cl V, and Ar VI of the aluminum sequence.

Highly ionized atoms have received much attention in plasma physics. Recent successes in fusion research with magnetically confined plasmas have made possible detailed spectral observations of the plasmas. These investigations have revealed the presence of highly ionized impurities which are released from the walls of the vessels as a result of intense bombardment by plasma particles. Atomic oscillator strengths are needed to determine the concentrations of the various impurities as well as their effects on the plasma (Wiese and Younger, 1976).

Lowly or medium ionized atoms are of astrophysical interest; for example, the spectra of quasi-stellar objects are now generally interpreted as

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red-shifted absorption and emission lines of lowly and medium ionized atoms (Nussbaumer, 1977). A knowledge of the OOS is important for the determination of astrophysical abundances.

2. ANALYTIC POTENTIAL MODEL

The potential for the active electron in an aluminumlike ion with nuclear charge Z is assumed to have the form

$$V(r)=-(2/r)\left\{12\left[H(e^{r/d}-1)+1\right]^{-1}+Z-12\right\} \tag{1}$$

where r is the electron–nucleus distance expressed in Bohr radii, and $V(r)$ is expressed in Rydbergs. This potential is a particular case of a more general form (Green et al., 1969) which has been used to characterize electron–atom interactions. The quantities d, H in Equation (1) are free parameters which may be adjusted to a selected body of experimental data. The potential given by Equation (1) is inserted into the radial Schrödinger equation

$$\left(\frac{d^2}{dr^2}-\frac{l(l+1)}{r^2}-V(r)+E_{nl}\right)P_{nl}(r)=0 \tag{2}$$

which is solved numerically by a Noumerov method to obtain the energy eigenvalues E_{nl} and wave functions $P_{nl}(r)/r$. The parameters d, H are determined by requiring the energy eigenvalues to agree with the experimental energy levels of the valence electron, which are obtained from the tables of Moore (Moore, 1958). The experimental levels are given in Table I.

An automatic search for the best parameters was performed using a least-squares search routine which adjusts the parameters in such a way as to minimize the quantity

$$\sum_i\left[w(E_e-E_c)^2\right]_i \tag{3}$$

Here E_e and E_c are the experimental and computed energies, respectively, and w is the weight. We use $w=E_e^{-1}$ in this work. Basically the search routine refines the values of the parameters through successive iterations which progressively reduce the value of the quantity (3) until it is minimized. The final values of the parameters are given in Table II. The computed levels, which are given in Table I, agree with the experimental levels to within 4% in all cases.

It may be noted that the potential parameters exhibit a systematic trend along the isoelectronic sequence. We find that the quantities

TABLE I. Experimental and Computed Energy Levels of P III, S IV, Cl V, and Ar VI (Units are Rydbergs)

Ion	Level	Experimental	Computed
P III	3*p*	−2.217	−2.212
	4*s*	−1.143	−1.140
	5*s*	−0.613	−0.617
	6*s*	−0.384	−0.387
	4*p*	−0.928	−0.949
	3*d*	−1.152	−1.164
	4*d*	−0.646	−0.640
	5*d*	−0.390	−0.401
	6*d*	−0.267	−0.274
	4*f*	−0.589	−0.565
	5*f*	−0.368	−0.362
	6*f*	−0.254	−0.251
	5*g*	−0.360	−0.360
	6*g*	−0.250	−0.250
	7*g*	−0.184	−0.184
S IV	3*p*	−3.477	−3.484
	4*s*	−1.824	−1.821
	5*s*	−1.007	−1.013
	4*p*	−1.530	−1.566
	3*d*	−2.091	−2.108
	4*d*	−1.150	−1.146
Cl V	3*p*	−4.985	−4.985
	4*s*	−2.649	−2.634
	3*d*	−3.291	−3.301
	4*d*	−1.800	−1.785
	5*d*	−1.130	−1.114
Ar VI	3*p*	−6.712	−6.711
	4*s*	−3.593	−3.576
	3*d*	−4.720	−4.732
	4*d*	−2.568	−2.555
	5*d*	−1.651	−1.595

TABLE II. Potential parameters for P III, S IV, Cl V, and Ar VI

Ion	d	H
P III	0.4495	1.2826
S IV	0.3840	1.1907
Cl V	0.3352	1.1222
Ar VI	0.2974	1.0692

d^{-1}, Hd^{-1} have a linear dependence on Z:

$$d^{-1}=0.3795Z-3.4678 \qquad (4)$$

$$Hd^{-1}=0.2474Z-0.8576 \qquad (5)$$

Equations (4) and (5) may be useful for extrapolating outside the range of the present calculations.

In nuclear phenomenology one assumes the existence of an analytic nuclear potential containing several adjustable parameters which are tuned to experimental data. The present approach, which assumes an analytic form for the electron–atom potential containing only two adjustable parameters, resembles this approach in nuclear physics.

3. RESULTS AND DISCUSSIONS

Using the wave functions corresponding to the eigenvalues in Table I, we have computed the OOS for the transitions $3s^2 3p(^2P_{1/2})$–$3s^2 ns(^2S_{1/2})$, $4 \leq n \leq 7$, and $3s^2 3p(^2P_{1/2})$–$3s^2 nd(^2D_{3/2})$, $3 \leq n \leq 7$. The results are presented in Table III. The computations are based upon the first Born approximation and the Russell–Saunders LS-coupling scheme for the initial and final states. The formulas which we use to compute the OOS are quite standard and may be found in various sources (Shore and Menzel, 1968). From Table III it can be seen that the $3p$–$3d$ transition dominates the OOS values in all the ions.

In Table IV we compare the present results with experimental and theoretical data. For the $3p$–$4s$ transition throughout the isoelectronic sequence, the present results are quite close to values which have been

TABLE III. Computed OOS for the Transitions $3s^2 3p(^2P_{1/2})$–$3s^2 ns(^2S_{1/2})$, $4 \leq n \leq 7$, and $3s^2 3p(^2P_{1/2})$–$3s^2 nd(^2D_{3/2})$, $3 \leq n \leq 7$, in P III, S IV, Cl V, and Ar VI

Z	$4s$	$5s$	$6s$	$7s$	
15	0.0863	0.0143	0.0053	0.0026	
16	0.0809	0.0140	0.0053	0.0026	
17	0.0767	0.0138	0.0052	0.0026	
18	0.0732	0.0134	0.0051	0.0026	
Z	$3d$	$4d$	$5d$	$6d$	$7d$
15	0.8555	0.0273	0.0032	0.00065	0.00018
16	0.8172	0.00039	0.0013	0.0016	0.0013
17	0.7484	0.0081	0.0100	0.0067	0.0045
18	0.6801	0.0301	0.0210	0.0124	0.0077

TABLE IV. Comparison between the Present Values of OOS and the Values from Experiment and Other Calculations for P III, S IV, Cl V, and Ar VI

Ion	$3p$ to	This calculation	Other calculations	Experiment
P III	$4s$	0.0863	0.098[a]	
	$3d$	0.8555		0.97 ± 0.10[b]
S IV	$4s$	0.0809	0.094[a]	
	$3d$	0.8172		0.91 ± 0.15[c]
Cl V	$4s$	0.0767	0.091[a]	
Ar VI	$4s$	0.0732	0.088[a]	

[a] Gruzdev and Prokofev (1966).
[b] Livingston et al. (1975).
[c] Irwin and Livingston (1976).

obtained by using the Coulomb approximation (Gruzdev and Prokofev, 1966). For the $3p$–$3d$ transition in P III and S IV, the present values are in good agreement with the experimental data (Livingston et al., 1975; Irwin and Livingston, 1976). These arguments suggest that the analytic potential model method is a realistic approach for calculating atomic oscillator strengths and other atomic properties. To the extent that the present work is an application of nuclear phenomenology to atomic physics, it is a contribution towards the unification of atomic physics and nuclear physics.

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