

## Excitation energies of $3p^6 3d^2 D \rightarrow 3p^5 3d 4s^4 P^0, ^4 D^0, ^4 F^0$ transitions in the potassium isoelectronic sequence

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**Abstract.** Excitation energies of  $3p^6 3d^2 D \rightarrow 3p^5 3d 4s^4 P^0, ^4 D^0$ , and  $^4 F^0$  transitions in  $\text{Cr}^{5+}$ ,  $\text{Mn}^{6+}$ ,  $\text{Fe}^{7+}$ ,  $\text{Co}^{8+}$ ,  $\text{Cu}^{10+}$  and  $\text{Zn}^{11+}$  ions of the potassium isoelectronic sequence have been calculated using Hartree-Fock as well as configuration interaction wavefunctions within the L-S coupling framework. A comparison with available experimental data shows good agreement between measurements and theoretical predictions.

**Keywords.** Hartree-Fock; configuration-interaction; excitation energies.

### 1. Introduction

In our recent extensive theoretical investigations (Tiwary 1982; Hibbert *et al* 1982; Tiwary 1983a, b, c, d; Tiwary *et al* 1983a, b) of the excitation energies and oscillator strengths of  $3p^6 3d^2 D \rightarrow 3p^5 3d^2 ^2 P^0, ^2 D^0, ^2 F^0$  and  $3p^6 3d^2 D \rightarrow 3p^5 3d 4s^2 P^0, ^2 D^0, ^2 F^0$  in  $\text{Sc}^{2+}$ ,  $\text{Ti}^{3+}$ ,  $\text{V}^{4+}$ ,  $\text{Cr}^{5+}$ ,  $\text{Mn}^{6+}$ ,  $\text{Fe}^{7+}$ ,  $\text{Co}^{8+}$ ,  $\text{Cu}^{10+}$  and  $\text{Zn}^{11+}$  ions of the potassium isoelectronic sequence, we have established that the inclusion of electron correlation is indispensable for obtaining reliable values of the excitation energies and oscillator strengths. We have also examined the effect of correlation on the positions of quartet states arising due to the excited configuration *i.e.* the  $3p^5 3d^2 ^4 S^0, ^4 P^0, ^4 D^0, ^4 F^0$  and  $^4 G^0$  states. Our results reflect a substantial effect of correlation of the quartet state energy. Recently, we studied the effect of correlation on the quartet states arising due to  $3p^5 3d 4s^4 P^0, ^4 D^0$  and  $^4 F^0$  in  $\text{Sc}^{2+}$ ,  $\text{Ti}^{3+}$  and  $\text{V}^{4+}$  ions. It was noticed that the correlation effect is not as important as the quartet states generated due to  $3p^5 3d^2$ .

In order to complete our earlier study of  $3p^6 3d^2 D \rightarrow 3p^5 3d 4s^4 P^0, ^4 D^0$  and  $^4 F^0$  transitions in the potassium sequence, we report here the excitation energies of quartet states arising due to  $3p^5 3d 4s$  in  $\text{Cr}^{5+}$ ,  $\text{Mn}^{6+}$ ,  $\text{Fe}^{7+}$ ,  $\text{Co}^{8+}$ ,  $\text{Cu}^{10+}$  and  $\text{Zn}^{11+}$  ions.

### 2. Theory

We represent the atomic state wavefunctions by the configuration interaction expansion as follows:

$$\Psi(LS) = \sum_{i=1}^M a_i \Phi_i(\alpha_i LS), \quad (1)$$

where  $L$  and  $S$  are the total orbital angular and spin quantum numbers of the state respectively,  $\alpha_i$  defines the angular momentum coupling scheme of the  $i$ th configu-

ation. The configurational wavefunctions  $\{\Phi_i\}$  are constructed from a set of one-electron functions, each of which consists of a product of a radial function, a spherical harmonic and a spin function:

$$U_{nlml}(\mathbf{r}, m_s) = \frac{1}{r} P_{nl}(r) Y_{lml}(\theta, \phi) X(m_s). \quad (2)$$

In order to preserve the orthonormality of these functions, we require

$$\int_0^\infty P_{nl}(r) P_{n'l}(r) dr = \delta_{nn'}; l+1 < n' < n. \quad (3)$$

We have expanded the radial wavefunctions in terms of analytic Slater-type orbitals,

$$P_{nl}(r) = \sum_{i=1}^K C_{jni} r^{l+jn} \exp(-\xi_{jni} r) \quad (4)$$

The theory is discussed in detail in our earlier work (see Tiwary *et al* 1983a).

### 3. Results and discussion

Table 1 gives the excitation energies of  $3p^6 3d^2 D \rightarrow 3p^5 3d 4s^4 P^0, ^4D^0$  and  $^4F^0$  transitions in  $\text{Cr}^{5+}, \text{Mn}^{6+}, \text{Fe}^{7+}, \text{Co}^{8+}, \text{Cu}^{10+}$  and  $\text{Zn}^{11+}$  ions of the potassium isoelectronic sequence. The configurations  $3p^5 3d^2$  and  $3p^5 3d 4s$  interact strongly in the case of  $^2L$  spectrum especially in lowly ionized ions *i.e.*  $\text{Sc}^{2+}, \text{Ti}^{3+}$  and  $\text{V}^{4+}$  ions. There is a fragmentation or distribution of oscillator strengths due to strong perturbation. In the case of  $^4L$  states, our calculations indicate that the mixing between  $3p^5 3d^2$  and  $3p^5 3d 4s$  is not significantly large implying that the separation between levels corresponding to  $3p^5 3d^2$  and  $3p^5 3d 4s$  is large. Ekberg (1973) has measured the energies of  $^4D$  and  $^4F$  states for  $\text{Cr}^{5+}$  ion. From table 1, it is clear that our theoretical

**Table 1.** Excitation energies of  $3p^6 3d^2 D \rightarrow 3p^5 3d 4s^4 P^0, ^4D^0, ^4F^0$  transitions in potassium sequence.

	$^4P^0$	$^4D^0$	$^4F^0$
$\text{Cr}^{5+}$	HF <sup>b</sup> 2.691	2.912	2.750
	CI <sup>c</sup> 2.612	2.804	2.680
	—	2.775 <sup>a</sup>	2.671 <sup>a</sup>
$\text{Mn}^{6+}$	HF 3.210	3.452	3.325
	CI 3.181	3.391	3.256
$\text{Fe}^{7+}$	HF 3.912	4.131	3.989
	CI 3.821	4.043	3.900
$\text{Co}^{8+}$	HF 4.511	4.801	4.613
	CI 4.469	4.713	4.556
$\text{Cu}^{10+}$	HF 5.998	6.289	6.123
	CI 5.956	6.231	6.054
$\text{Zn}^{11+}$	HF 6.812	7.121	6.902
	CI 6.774	7.066	6.872

a) Ekberg (1973): Experimental values  
 b) Hartree-Fock (HF) c) Configuration-interaction (CI)

predictions are in good agreement with the experimental observations. Similar calculations have been performed for all other ions. It is expected that the correlation effect will be smaller for highly ionized atoms and hence we believe that our results will be reliable for all ions.

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