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Radiative transitions in highly ionised silicon-like ions

B. Saha[1], A.K. Das[1,a], and P.K. Mukherjee[1,2]

[1] Department of Spectroscopy, Indian Association for the Cultivation of Science, Jadavpur, Calcutta 700 032, India
[2] Max-Planck Institut für Astrophysik, Karl-Schwarzschild strasse 1, 85740 Garching, Germany

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Abstract. Transition energies, oscillator strengths and transition probability values for radiative transitions have been calculated for the highly ionised atoms of Si isoelectronic sequence from Mn^{11+} to Kr^{22+} for the singly excited states up to principal quantum number $n = 7$. Time-dependent coupled Hartree-Fock (TDCHF) theory has been used to estimate such transition properties. Most of the results for the oscillator strengths and transition probabilities are new. Transition energies agree reasonably well with available spectroscopic values.

PACS. 31.50.+w Excited states – 32.70.Cs Oscillator strengths, lifetimes, transition moments

1 Introduction

The study of radiative transition properties of highly ionised atoms is of considerable interest in recent years because of their importance in the diagnostic determination and modeling of high temperature astrophysical and laboratory plasma [1–3] and in calculating stellar envelope opacities [4]. In this context such studies for highly stripped Si like ions are important as many of these ions have been observed in solar corona, in tokamak discharges and in laser produced plasma. Si like Fe^{12+} lines have been detected in solar corona by Widing *et al.* [5], Malinovsky and Heroux [6] and Behring *et al.* [7] and in laboratory plasma by Fawcett [8]. Fawcett and his coworkers [9,10] observed and analysed the spectra of Ni^{13+} and Co^{14+} originating from radiative transitions from their excited configurations $3s3p^3$, $3s^23p3d$, $3s^23p4d$ and $3s^23p4s$. Kastner *et al.* [11] analysed the wavelengths corresponding to the transition $3p^2 \rightarrow 3p4d$ in Si like Cr^{10+} to Zn^{16+} and Johansson [12] identified lines corresponding to radiative and intercombination lines of S^{2+} with vacuum spark spectra. Experiment on laser produced plasma by Khan [13] on Si like Cu^{15+} and Zn^{16+} yields the wavelengths for $3p^2 \rightarrow 3p4s$ and $3p4d$ transitions. Si like Cu^{15+} to Mo^{28+} ions generated by Tokamak experiment due to Sugar *et al.* [14] give data for the allowed and intercombination lines connected with the transitions $3s^23p^2 \rightarrow 3s3p^3$ and $3s^23p4d$. Similar experiments by Wyart and TFR group [15] and by Jupén *et al.* [16] identified wavelengths corresponding to the transitions $3p^2 \rightarrow 3p3d$ and $3s^23p^2 \rightarrow 3s3p^3$ for several Si like ions from Ti^{8+} to Rh^{31+}. Systematic analysis of the intercombination lines of several ions of Si isoelectronic sequence was performed by Träbert [17,18] and his coworkers [19–22]. Details of such studies on Si isoelectronic series may be obtained from the compilation of Sugar and Corliss [23] and Shirai *et al.* [24–27].

A number of theoretical estimates using different techniques exist for the transition properties within ground configuration, intercombination lines and radiative transitions for $n = 3$ to $n = 4$. The important ones are the multiconfiguration Dirac Fock (MCDF) calculation of energy levels, oscillator strengths and transition probabilities for Si like ions from $Z = 15$ to $Z = 106$ by Huang [28], relativistic Hartree Fock calculation (HFR) with configuration interaction (CI) of Fawcett [29] for $Z = 14$ to $Z = 28$, the MCDF calculation of Khostall *et al.* [30] for $Z = 16$ to $Z = 36$, the HXR calculation by Biémont [31] and by Biémont and Bromage [32] for several such ions. Recent data bases [33,34] in this regard yield more information. Very recently Nahar [35] used R matrix close coupling method for the estimation of oscillator strengths and transition probabilities for the fine structure levels in Si like Fe^{12+} from ground to excited levels covering $n = 4$.

In this paper we present some data on the radiative transition properties for Si like ions from Mn^{11+} to Kr^{22+} for the transitions $3p^2\ {}^3P \rightarrow 3pns\ {}^3P^0$ and $3pnd\ {}^3D^0$, $n \leq 7$. We used time dependent coupled Hartree Fock (TDCHF) method under LS coupling scheme. The transition energies and other properties like the oscillator strengths and transition probabilities are extracted from a study of the position of poles of an appropriately constructed linearised variational functional discussed in detail earlier [36,37]. The present theory includes partial correlation effects to the extent of hole particle correlations to all orders in perturbation theory [38,39] and provides reasonable estimates of transition properties [40,41]. An outline of the theory is presented in Section 2 and results are discussed in Section 3.

[a] e-mail: sppkm@mahendra.iacs.res.in
or e-mail: spakd@mahendra.iacs.res.in

2 Method

The Si isoelectronic sequence of ions is described by the usual nonrelativistic Hamiltonian H_0 (we use atomic units throughout). An external oscillatory perturbation of the form

$$H'(\bar{r},t) = G(\bar{r})\mathrm{e}^{\mathrm{i}wt} + \text{complex conjugate} \tag{1}$$

is applied on the system. $G(\bar{r})$ is a symmetric sum of one-particle operators which initiates multipolar excitations

$$G(\bar{r}) = \lambda \sum_i r_i^l P_l(\cos\theta_i). \tag{2}$$

In the present context, we consider only dipolar perturbation for which $l = 1$. We assume the perturbation strength parameter λ to be small so that linear response approximation is valid and the perturbation admixes first order oscillatory corrections $\delta\Psi_i^{\pm}$ to the ground state wave functions Ψ_i. A variational functional of the form

$$J(\Phi) = \frac{1}{T}\int_0^T \frac{\langle\Phi|H - \mathrm{i}\partial/\partial t|\Phi\rangle}{\langle\Phi|\Phi\rangle}\mathrm{d}t \tag{3}$$

is constructed to obtain the first-order correction from the optimization condition

$$\delta J(\Phi) = 0 \tag{4}$$

where the optimization is done with respect to suitable linear variation parameters introduced in the basis functions. Φ denotes the total wave function and H is the total Hamiltonian in the presence of the external perturbation. Behaviour of the functional J with respect to external frequency ω is studied by calculating the frequency dependent dipole polarisability $\alpha_\mathrm{d}(\omega)$. The polarisability $\alpha_\mathrm{d}(\omega)$ passes through poles at certain characteristic frequencies which correspond to the transition energies of the system to its various excited states. Renormalised first order perturbation functions at pole positions furnish the excited state wave functions. These are subsequently used to estimate the oscillator strengths, transition probabilities and other properties connected with a specific transition.

3 Results and discussions

Presently we have studied the low and relatively higher lying radiative $p \rightarrow s$ and $p \rightarrow d$ transitions for the highly stripped ions of Si isoelectronic sequence from Mn^{11+} to Kr^{22+}. The transitions considered are $3p^2\ {}^3\mathrm{P} \rightarrow 3p(^2\mathrm{P})\,ns\ {}^3\mathrm{P}^0$ and $3p^2\ {}^3\mathrm{P} \rightarrow 3p(^2\mathrm{P})nd\ {}^3\mathrm{D}^0$ $(n = 4, ..., 7)$. The ground state functions are taken from Clementi and Roetti [42]. The radial part of the first order perturbed functions is taken as linear combinations of Slater bases (STO)

$$\delta\Psi_i^{\pm}(r) = \sum_k C_{ik}^{\pm}\chi_{ik}(r) \tag{5}$$

where $C_{ik}^{\pm}$ are linear variation parameters due to two components of the harmonic perturbation. The angular part of $\delta\Psi_i^{\pm}$ is determined by the nature of the angular part of the perturbing operator and the orbital Ψ_i on which it acts. The radial basis set is of the form

$$\chi_{ik}(r) \approx r^{n_{ik}}\mathrm{e}^{-\rho_{ik}r} \tag{6}$$

where the exponents n_{ik} and ρ_{ik} are preassigned from physical considerations. In the present case the number of parameters has been fixed to 15 for all the excitations. This gives convergence within a preassigned static limit of the frequency-dependent dipole polarisability values.

In Table 1, transition energies, oscillator strengths and transition probability values for the transitions $3p^2\ {}^3\mathrm{P} \rightarrow 3pns\ {}^3\mathrm{P}^0$ and $3p^2\ {}^3\mathrm{P} \rightarrow 3pnd\ {}^3\mathrm{D}^0$ $(n \leq 7)$ for Si isoelectronic ions under study have been displayed. Only the excited orbitals connected with the transitions are shown in the table. The oscillator strengths and transition probability values have been evaluated using well known formulae [40,43]. We have used LS coupling scheme to designate the energy levels and compare them with the available spectroscopic values of Shirai *et al.* [24–27]. It is observed that for Fe^{12+} the deviations lie within 0.5% and 0.07% with the values listed by Shirai *et al.* [26]. For ions like Co^{13+} to Cu^{15+}, our results lie within 0.5% compared to experimental values. It is also observed that the deviation of $4s$ energy levels is much less than that of the $4d$ levels. This is possibly due to mixing of higher configurations which affect the d levels more than the s levels. With increase of nuclear charge the errors are likely to be less as the effect of electron correlation diminishes along higher members of the isoelectronic series. We are unable to find the $3p \rightarrow 3d$ excitation for all the ions. The reason being that excitation energies for the $4s$ levels in these ions and also the intra shell excitation $3s^23p^2\ {}^3\mathrm{P} \rightarrow 3s3p^3\ {}^3\mathrm{P}^0$ fall pretty close to the $3d$ excitation energies. Mixing of these configurations in the wave function is necessary to get the $3d$ excitation energies. In fact we notice that the shell-wise contribution from the $3s$ shell to $\alpha_\mathrm{d}(\omega)$ is very large and it changes much faster than contributions from other shells around the region of excitation concerned. The total polarisability shows oscillatory behaviour in this region thus effectively preventing closer studies. The $3p \rightarrow 7s$ transition in As^{19+} and Se^{20+} is also suppressed by the $3s$ shell contribution near the transition $3s \rightarrow np$. A few other transition energies available for comparison for the $4s$ and $4d$ excitations show reasonable agreement with our computed values. Very few results are available for the oscillator strengths and transition probability values for excitations from the ions under study. For Fe^{12+} our result 0.152 for the oscillator strength for the $3p \rightarrow 4s$ transition is appreciably higher than that of 0.088 due to Shirai [26] and 0.062 and 0.10 due to Nahar [35], the transition probability value is also larger than that of Shirai [26]. The oscillator strength for the $3p \rightarrow 4d$ transition for Fe^{12+} is larger than that calculated by Nahar [35] and the same pattern is followed for the transition probability value for Fe^{12+} and Zn^{16+} when compared with that of Kastner [11]. While we note that the previous values have some

Table 1. Transition energies (a.u.), Oscillator strengths and Transition probabilities (s^{-1}) for the radiative transitions in highly ionised Si like ions.

Ion	State	Transition energy		Oscillator strength		Transition probability	
		Present calc.	Other values	Present calc.	Other values	Present calc.	Other values
Mn^{11+}	$4s\ ^3P^0$	5.3283		0.155		1.40(+11)*	
	5*s*	7.8121		0.308(-1)		6.01(+10)	
	6*s*	9.0444		0.283(-1)		7.40(+10)	
	7*s*	9.7817		0.104(-1)		3.17(+10)	
	$4d\ ^3D^0$	6.4211	6.4428[a]	0.505		6.65(+11)	
	5*d*	8.3184		0.160		3.53(+11)	
	6*d*	9.3158		0.655(-1)		1.82(+11)	
	7*d*	9.9136		0.520(-1)		1.63(+11)	
Fe^{12+}	$4s\ ^3P^0$	6.0922	6.0878[b]	0.152	0.088[b]	1.80(+11)	1.0(+11)[b]
					0.062[c]		
					0.10[d]		
	5*s*	8.9328		0.308(-1)		7.86(+10)	
	6*s*	11.1571		0.850(-2)		4.29(+10)	
	7*s*	11.6825		0.169(-2)		0.74(+10)	
	$4d\ ^3D^0$	7.2748	7.3073[a]	0.556	0.361[c]	9.39(+11)	1.96(+11)[a]
			7.2366[b]		0.346[d]		
	5*d*	9.4854		0.171		4.92(+11)	
	6*d*	10.6484		0.732(-1)		2.65(+11)	
	7*d*	11.3433		0.565(-1)		2.32(+11)	
Co^{13+}	$4s\ ^3P^0$	6.9050	6.8983[b]	0.149		2.27(+11)	
	5*s*	10.1260		0.307(-1)		1.00(+11)	
	6*s*	11.7327		0.740(-2)		3.25(+10)	
	7*s*	12.6539		0.668(-2)		3.42(+10)	
	$4d\ ^3D^0$	8.1772	8.3726[a]	0.602		1.29(+12)	
			8.1333[b]				
	5*d*	10.7233		0.181		0.66(+12)	
	6*d*	12.0634		0.770(-1)		0.36(+12)	
	7*d*	12.8717		0.552(-1)		0.29(+12)	
Ni^{14+}	$4s\ ^3P^0$	7.7669	7.7609[b]	0.145		2.83(+11)	
	5*s*	11.3881		0.301(-1)		1.25(+11)	
	6*s*	13.2068		0.861(-2)		0.48(+11)	
	7*s*	14.2717		0.547(-2)		0.36(+11)	
	$4d\ ^3D^0$	9.1282	9.1899[a]	0.646		1.72(+12)	
			9.0814[b]				
	5*d*	12.0334		0.189		0.88(+12)	
	6*d*	13.5646		0.820(-1)		0.48(+12)	
	7*d*	14.4797		0.617(-1)		0.41(+12)	
Cu^{15+}	$4s\ ^3P^0$	8.6775	8.6446[b]	0.144		3.47(+11)	
			8.6213[e]				
	5*s*	12.7243		0.297(-1)		1.54(+11)	
	6*s*	14.7679		0.927(-2)		0.65(+11)	
	7*s*	15.9670		0.575(-2)		0.47(+11)	
	$4d\ ^3D^0$	10.1279	10.2092[a]	0.685		2.24(+12)	
			10.0753[b]				
			10.0782[e]				
	5*d*	13.4147		0.197		1.13(+12)	
	6*d*	15.1481		0.854(-1)		0.63(+12)	
	7*d*	16.1789		0.661(-1)		0.55(+12)	
Zn^{16+}	$4s\ ^3P^0$	9.6370	9.5241[e]	0.143		4.24(+11)	
	5s	14.1328		0.292(-1)		1.86(+11)	
	6s	16.4227		0.936(-2)		0.81(+11)	
	7*s*	17.7903		0.604(-2)		0.61(+11)	

Table 1. *Continued.*

Ion	State	Transition energy		Oscillator strength		Transition probability	
		Present calc.	Other values	Present calc.	Other values	Present calc.	Other values
Zn^{16+}	$4d\ ^3D^0$	11.1762	11.2837[a]	0.723		2.88(+12)	6.37(+11)[a]
			11.1457[e]				
	$5d$	14.8674		0.203		1.44(+12)	
	$6d$	16.8154		0.880(-1)		0.80(+12)	
	$7d$	17.9666		0.806(-1)		0.83(+12)	
Ga^{17+}	$4s\ ^3P^0$	10.6445		0.141		5.12(+11)	
	$5s$	15.6121		0.288(-1)		2.25(+11)	
	$6s$	18.1403		0.963(-2)		1.01(+11)	
	$7s$	19.6354		0.645(-2)		0.79(+11)	
	$4d\ ^3D^0$	12.2731		0.758		3.65(+12)	
	$5d$	16.3915		0.209		1.79(+12)	
	$6d$	18.5664		0.899(-1)		0.99(+12)	
	$7d$	19.8633		0.110(-1)		0.14(+12)	
Ge^{18+}	$4s\ ^3P^0$	11.7011		0.140		6.11(+11)	
	$5s$	17.1630		0.286(-1)		2.69(+11)	
	$6s$	19.9512		0.972(-2)		1.24(+11)	
	$7s$	21.6017		0.768(-2)		1.15(+11)	
	$4d\ ^3D^0$	13.4187		0.789		4.54(+12)	
	$5d$	17.9871		0.214		2.21(+12)	
	$6d$	20.4020		0.921(-1)		1.23(+12)	
	$7d$	21.8383		0.353(-1)		0.54(+12)	
As^{19+}	$4s\ ^3P^0$	12.8065		0.138		7.25(+11)	
	$5s$	18.7852		0.282(-1)		3.18(+11)	
	$6s$	21.8480		0.967(-2)		1.47(+11)	
	$4d\ ^3D^0$	14.6129		0.819		5.59(+12)	
	$5d$	19.6539		0.218		2.70(+12)	
	$6d$	22.3208		0.932(-1)		1.48(+12)	
	$7d$	23.9145		0.401(-1)		0.73(+12)	
Se^{20+}	$4s\ ^3P^0$	13.9606		0.137		8.51(+11)	
	$5s$	20.4792		0.280(-1)		3.74(+11)	
	$6s$	23.8283		0.974(-2)		1.77(+11)	
	$4d\ ^3D^0$	15.8557		0.846		6.79(+12)	
	$5d$	21.3918		0.233		3.25(+12)	
	$6d$	24.3234		0.950(-1)		1.80(+12)	
	$7d$	26.0697		0.443(-1)		0.96(+12)	
Br^{21+}	$4s\ ^3P^0$	15.1635		0.135		9.94(+11)	
	$5s$	22.2448		0.276(-1)		4.37(+11)	
	$6s$	25.9042		0.973(-2)		2.09(+11)	
	$7s$	28.1064		0.277(-2)		0.70(+11)	
	$4d\ ^3D^0$	17.1472		0.871		8.18(+12)	
	$5d$	23.2007		0.226		3.89(+12)	
	$6d$	26.4105		0.955(-1)		2.13(+12)	
	$7d$	28.3345		0.449(-1)		1.15(+12)	
Kr^{22+}	$4s\ ^3P^0$	16.4147		0.134		1.15(+12)	
	$5s$	24.0795		0.275(-1)		0.51(+12)	
	$6s$	28.0357		0.966(-2)		0.24(+12)	
	$7s$	30.4049		0.292(-2)		0.86(+11)	
	$4d\ ^3D^0$	18.4873		0.894		9.76(+12)	
	$5d$	25.0817		0.230		4.62(+12)	
	$6d$	28.5792		0.975(-1)		2.55(+12)	
	$7d$	30.6650		0.474(-1)		1.42(+12)	

* x(+n)=x*10^{+n}, [a]: Ref. [11], [b]: Ref. [24–27], [c]: Ref. [35], [d]: Value quoted in Ref. [35], [e]: Ref. [13].

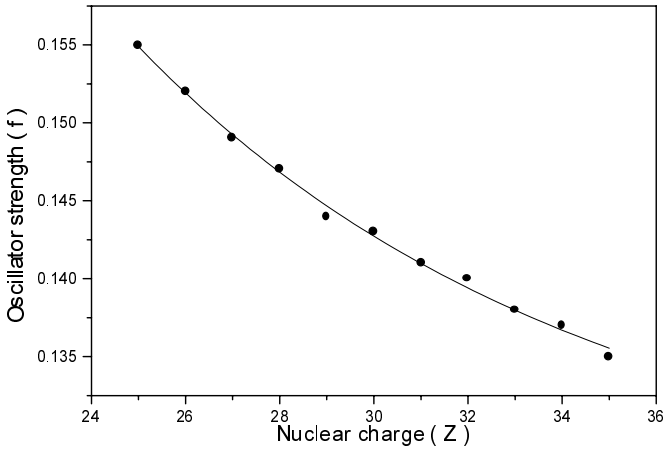

Fig. 1. Plot of oscillator strength (f) *vs.* Z for $3p \rightarrow 4s$ transitions of highly stripped Si-like ions.

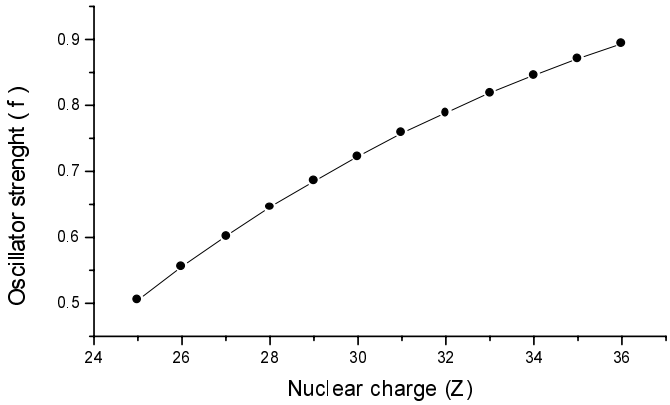

Fig. 2. Plot of oscillator strength (f) *vs.* Z for $3p \rightarrow 4d$ transitions of highly stripped Si-like ions.

uncertainties our results also are affected by uncertainties due to the cancellation effects from strong mixing of the levels $3s3p^3$ and $3s^23p3d$ [18]. The effect is more for the $3p \rightarrow 4s$ transition as reflected in the plot of the oscillator strength against nuclear charge in Figure 1 which shows a scatter of the data along a mean curve. Similar plot for the $3p \rightarrow 4d$ oscillator strengths in Figure 2 shows more systematic behaviour. The nodal structure of the functions is also responsible for the value of the transition matrix elements which affects the oscillator strength directly. For ions with larger Z the order of the transition probability is in agreement with that predicted by Cowan [44].

In view of the paucity of atomic data available for higher excitations in Si isoelectronic ions, we believe, our reported data may serve as a useful set for future reference.

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