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Theoretical calculations of the energies of the K_α satellite and hypersatellite lines of magnesium

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Abstract. The satellite and hypersatellite x-ray lines which lie on the high energy side of the dipole $K_{\alpha_{1,2}}$ lines are generally attributed to multiple ionization. In this paper, an attempt is made to calculate the energies of these lines in the x-ray spectrum of the magnesium atom using screened hydrogenic wavefunctions. Besides the good agreement found between our calculated values and the experimental results, our calculations give some additional lines not reported earlier.

Keywords. X-ray emission spectra; multiple ionisation; satellite lines; hypersatellite lines; screened hydrogenic wavefunctions.

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1. Introduction

It is well known (Deodhar 1962; Richard 1974; Jamison *et al* 1975; Ḱeski-Rahkonen *et al* 1977; Armour *et al* 1980; Aberg and Suvanen 1982) that x-ray emission lines are often accompanied on their high energy side by several weak lines called satellite or non-diagram lines. These lines, unlike the forbidden lines (Edlabadkar and Mande 1983), cannot be explained with the help of normal energy level diagrams and hence the name non-diagram lines is given to them. Their origin and interpretation have not yet been fully understood. It is important to understand the mechanisms which cause the emission of such lines, since they can help in obtaining a better insight into the different processes occurring in the inner shells of atoms. The non-diagram lines, generally attributed to multiple ionizations produced by different mechanisms, such as bombardment with heavy ions, K capture resulting in a shake-off etc (Richard *et al* 1973; Briand *et al* 1971; Sagawa 1971), lying in the range 0–100 eV from the parent lines are called satellite lines, while those which lie beyond this region are called hypersatellite lines. The K_α satellite lines are usually attributed to the transitions of electrons in the $2p$ shell to a singly-ionized $1s$ shell in the presence of spectator vacancies in the L shell, while the K_α hypersatellite lines are attributed to similar transitions to the $1s$ shell which is initially doubly-ionized. In the present work, an attempt is made to calculate the energies of the satellite and hypersatellite lines of magnesium lying on the high energy side of the $K_{\alpha_{1,2}}$ lines using screened hydrogenic wavefunctions.

2. Procedure for calculations

For calculating the average energies of the magnesium atom in different configurations with the help of screened hydrogenic wavefunctions, we have obtained the screening constants using an approximation (Slater 1960) according to which the radius of maximum charge density of an electron in an orbital in a multielectron atom is equal to the radius of the corresponding orbital of the electron in the hydrogen atom divided by $(Z-\sigma)$, σ is the screening constant. For obtaining the radii of the electronic orbits, we assume, following Tankhiwale *et al* (1971, 1972), that the electron in a particular orbital spends most of its time in the region of maximum charge density. The radii of maximum charge density for different orbitals of the hydrogen atom were obtained from their radial wave-functions (Condon and Shortley 1953). The values of r_{max} obtained by the SCF calculations for the different orbitals of magnesium were taken from Slater (1960). However, it may be mentioned that the Z_{eff} values thus obtained are for neutral atoms. Their numerical values for the magnesium atom are found to be 11·52, 9·25, 8·48 and 4·95 for the 1*s*, 2*s*, 2*p* and 3*s* orbitals respectively. Due to multiple ionisation, the screening gets reduced and to account for this, the screening values are suitably modified in the way described by Tankhiwale *et al* (1971). Our present calculation shows that, for magnesium the screening of a *K* shell electron by the other electron from the same shell comes out as 0·48, while the screening for an *L* electron by a single *K* electron and a single *L* electron is 0·75 and 0·30 respectively.

Since for light atoms, such as magnesium, the Russel-Saunder's coupling holds true (Condon and Shortley 1953), we have calculated the average energy of the different configurations using Slater's (1960) expression

$$E_{av} = \Sigma I(nl) + \Sigma(\text{pairs}) \text{ interaction energy}, \tag{1}$$

where $I(nl)$ is one electron integral.

For satellite calculations, the average energies of the magnesium atom with the initial configuration $1s^{-1}\,2p^{-n}$ with n ranging from 1 to 5 and final configuration $2p^{-n-1}$ were calculated from the above expression. Similar calculations were made for the hypersatellites taking the initial configuration to be $1s^{-2}\,2p^{-n}$ and the final configuration as $1s^{-1}\,2p^{-n-1}$. Besides these, we have also made calculations for the satellite lines assuming a permanent hole in the 2*s* shell and taking the initial configuration to be $1s^{-1}\,2s^{-1}\,2p^{-n}$ and for the hypersatellite lines taking the initial configuration as $1s^{-2}\,2s^{-1}\,2p^{-n}$.

The radial integrals, often called the Slater-Condon parameters, required for the calculations as given by Slater (1960) are

$$F^k(n_1l_1,n_2l_2) = e^2 \int_{r_1=0}^{\infty} \int_{r_2=0}^{\infty} R^2_{n_1l_1}(r_1) R^2_{n_2l_2}(r_2) \frac{(r_<)^k}{(r_>)^{k+1}} r_1^2 r_2^2 \mathrm{d}r_1\,\mathrm{d}r_2, \tag{2}$$

and

$$G^k(n_1l_1,n_2l_2) = e^2 \int_{r_1=0}^{\infty} \int_{r_2=0}^{\infty} R_{n_1l_1}(r_1) R_{n_2l_2}(r_1) \frac{(r_<)^k}{(r_>)^{k+1}} R_{n_1l_1}(r_2) R_{n_2l_2}(r_2) r_1^2 r_2^2 \mathrm{d}r_1 \mathrm{d}r_2, \tag{3}$$

where $R_{n_1l_1}$ and $R_{n_2l_2}$ are the radial parts of the hydrogenic wavefunctions.

To calculate the Slater-Condon parameters involving the 1*s*, 2*s* and 2*p* orbitals we have used normalized hydrogenic wavefunctions corrected for screening using our

screening parameters. Amongst them, $2p$ is orthogonal to $1s$ and $2s$ due to their angular parts, but $1s$ and $2s$ are not orthogonal to each other. From the non-orthogonal wavefunctions R_{1s} and R_{2s}, we generate the orthogonal wavefunctions R_{1s} and R'_{2s} using Schmidt orthogonalization process (Merzbacher 1970). We observe that our wavefunctions R_{1s}, R'_{2s}, R_{2p} are similar in form to the corresponding wavefunctions of Morse *et al* (1935), though the constants and coefficients are different because of the different Z_{eff} values used by us. Making use of these, we have calculated the values of the one-electron integrals and F's and G's using the tables of Morse *et al* as given by Slater (1960). The interaction energies of the $1s$, $3s$ and $2p$, $3s$ orbitals were found by evaluating the F and G integrals from equations (2) and (3), since these are not tabulated by Morse *et al* (1935). The $2p$ orbital is orthogonal to $3s$ due to thier angular parts. We have tried to avoid the lack of orthogonality of the $1s$ and $3s$ orbitals by considering a single effective charge Z^* equal to the geometric mean of the effective charges of the $1s$ and $3s$ orbitals, as has been done earlier by Assad and Burhop (1958).

3. Results and discussion

In table 1 we have compared our calculated energies for the satellite lines with the experimental energies and HFS calculations given by Richard *et al* (1973). Similarly in table 2 we have compared our calculated energies for the hypersatellite lines with the experimental energies and HFS calculations of Richard *et al* (1973). Our calculated values for the satellite as well as the hypersatellite lines are generally in good agreement with the experimental and theoretical values of Richard *et al*. In particular, it will be seen from table 2 that for the experimentally observed line at 1373 eV our calculated value 1374·3 eV is in much better agreement than the corresponding theoretical value

Table 1. Energies of the magnesium K_α satellite lines.

	Energy (eV)		
Initial configuration	Present calculations	Experimental energy (Richard *et al* 1973)	Calculated Values HFS (Richard *et al* (1973)
$1s^{-1}$	1254·1	1253·6	1254
$1s^{-1}\,2p^{-1}$	1260·5	1261·5	1262
$1s^{-1}\,2s^{-1}$	1263·2	1264	
$1s^{-1}\,2p^{-2}$	1270·9	1266·5	
		1270·7	1272
$1s^{-1}\,2s^{-1}\,2p^{-1}$	1273·4	1272	
		1273·3	
$1s^{-1}\,2p^{-3}$	1281·7	1281	1284
$1s^{-1}\,2s^{-1}\,2p^{-2}$	1283·0	1283	
$1s^{-1}\,2p^{-4}$	1296·1	1293	1298
$1s^{-1}\,2s^{-1}\,2p^{-3}$	1295·1	1295·4	
$1s^{-1}\,2p^{-5}$	1311·9		1313
$1s^{-1}\,2s^{-1}\,2p^{-4}$	1308·9	1307	
$1s^{-1}\,2s^{-1}\,2p^{-5}$	1326·0		

Table 2. Energies of the magnesium K_α hypersatellite lines.

Initial configuration	Energy (eV)		
	Present calculations	Experimental energy (Richard *et al* 1973)	Calculated Values HFS (Richard *et al* 1973)
$1s^{-2}$	1353		
$1s^{-2}\,2p^{-1}$	1363·3		
$1s^{-2}\,2s^{-1}$	1365·2		
$1s^{-2}\,2p^{-2}$	1374·3	1373	1364
$1s^{-2}\,2s^{-1}\,2p^{-1}$	1381·7	1378	
$1s^{-2}\,2p^{-3}$	1387·2	1388	1378
$1s^{-2}\,2s^{-1}\,2p^{-2}$	1395·0	1390	
$1s^{-2}\,2p^{-4}$	1404·1	1401	1392
$1s^{-2}\,2s^{-1}\,2p^{-3}$	1411·3		
$1s^{-2}\,2p^{-5}$	1421·9	1410	1409
$1s^{-2}\,2s^{-1}\,2p^{-4}$	1426·1	1414	
$1s^{-2}\,2s^{-1}\,2p^{-5}$	1444·8		

Note: The values of Aberg and Suvanen (1982) for the theoretically calculated energies of hypersatellites $K\alpha_2^h$ and $K\alpha_1^h$ corresponding to transitions $1s^{-2}(^1S_0) \rightarrow 1s^{-1}2p^{-1}(^1P_1)$ and $1s^{-2}(^1S_0) \rightarrow 1s^{-1}2p^{-1}(^3P_1)$ are 1368·8 eV and 1374·7 eV respectively.

given by Richard *et al*. So is the case with the experimental lines at 1388 eV and 1401 eV. The experimentally observed line at 1410 eV agrees very well with our calculated value for the transition with the initial state configuration $1s^{-2}\,2s^{-1}\,2p^{-3}$.

The positions of the satellite and hypersatellite lines are shown in figure 1 along with the theoretical and experimental values of Richard *et al* (1973). The figure clearly shows that our calculations give some additional lines not reported previously.

It may be noted that our calculations involving a permanent hole in the 2*s* shell explain several unaccounted experimental lines. In these transitions, in spite of a large L_1-L_2M Coster-Kroning transition rate (McGuire 1971), the intensity of the emitted

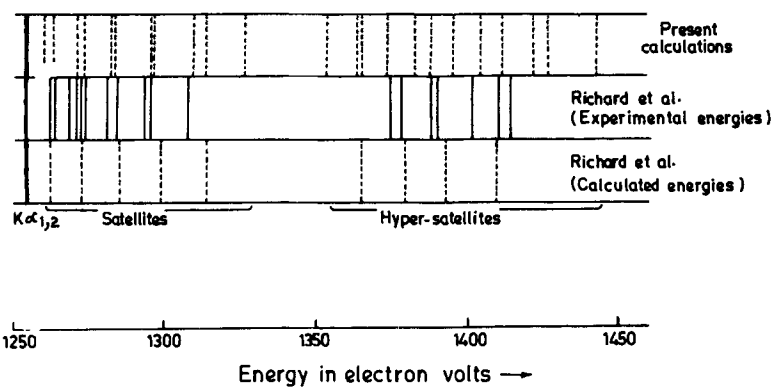

Figure 1. Positions of the magnesium K_α satellite and hypersatellite lines.

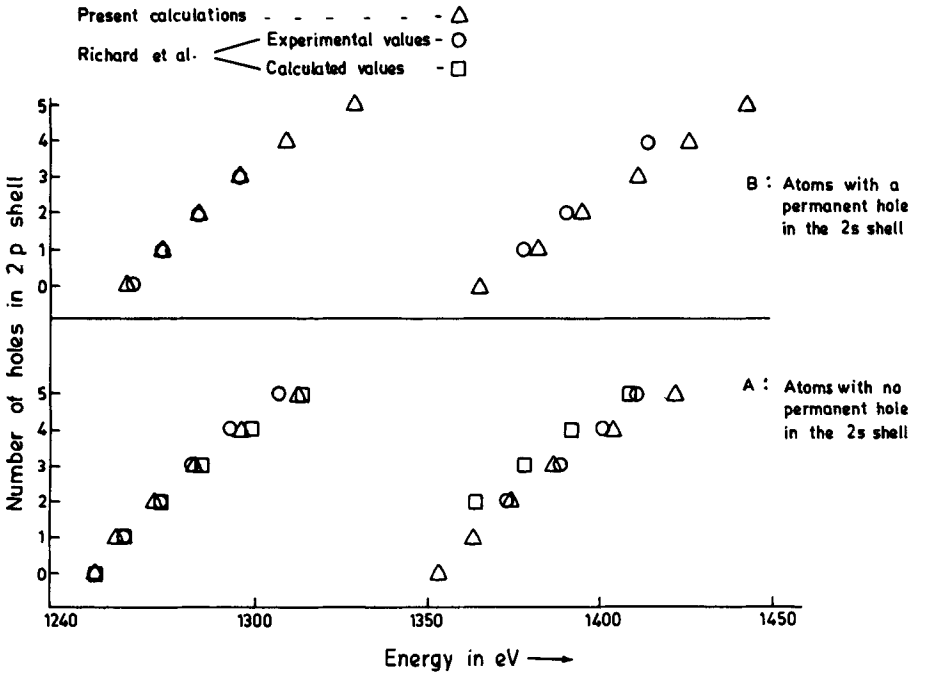

Figure 2. Variation of the energies of the magnesium K_α satellite and hypersatellite lines with the number of holes in the $2p$ shell.

radiations from atoms with a spectator vacancy in the $2s$ orbital is only 10% less than those from atoms with a spectator vacancy in the $2p$ orbital (Knudson *et al* 1971). Because of heavy ion impact the probability for vacancies in the $2s$ and $2p$ orbitals to be formed would be large so that one may expect that a much greater number of atoms get ionized in the $2s$ shell, resulting in intensity sufficient enough for these satellite and hypersatellite lines to be observed.

In figure 2 our calculated energies are plotted as a function of the number of $2p$ holes. Figure 2A refers to the case of atoms in which there is no permanent hole in the $2s$ shell while 2B depicts the case of atoms with a permanent hole in the $2s$ shell. Our calculated energies are compared in these figures with the theoretical and experimental values of Richard *et al* bringing out a very interesting parallelism between the satellite and hypersatellite lines.

It is interesting to note here that Armour *et al* (1980) carried out experimental work and theoretical calculations of x-ray satellite lines of highly ionized magnesium atom in which transitions take place from $1s$ to np with n ranging from three to ten. Their study is of importance in astrophysical and laboratory plasmas due to the availability of satellite-borne x-ray spectrometers and controlled thermonuclear fusion research.

It is worthwhile to mention here that in Auger electron spectra, the existence of satellite lines has been extensively reported following the initial observation of Körber and Mehlhorn (1966). These satellite lines may be divided into three groups, depending on whether they arise from atoms with (a) single hole in the ionized shell and holes in outer shells; (b) multiple vacancies in the innermost ionized shell while no other shell has holes and (c) multiple holes in both the innermost ionized shell and in the outer

shells. The three cases should lead to satellites, hypersatellites and satellites of hypersatellites respectively. Several studies have been reported on such satellites (Asaad and Burhop 1972; Carlson 1975; Crasemann 1975; Vayrynen *et al* 1983). However, not many theoretical calculations on satellites in Auger spectra seem to have been carried out so far.

4. Concluding remarks

As stated earlier, it is possible to obtain from the study of x-ray satellite and hypersatellite lines a better insight into the processes occurring in the inner shells of atoms as well as a better understanding of the ionisation processes. With the heavy ion bombarding facilities and synchroton sources now available for producing multiple ionized atoms and with the advent of high resolution spectroscopic techniques, it may now be worthwhile to carry out further studies of the x-ray satellite spectra to obtain information on the transient ionic configurations of atomic systems.

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