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CALCULATIONS OF RADIATIVE AND NON-RADIATIVE DECAY RATES FOR DOUBLY-EXCITED STATES IN HIGHLY IONIZED Ar

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ABSTRACT

Calculations are reported of radiative and non-radiative decay rates for doubly excited states of the type \(1s^2n\ell n'\ell'\) in Ar\(^{14+}\) with \(n\) and \(n'\) in the range 6 to 9. This type of configuration is expected to be formed in charge exchange collisions between Ar\(^{16+}\) and the neutral rare gases and the ratio between the radiative and the total decay rate is one of the experimentally accessible parameters. We show that the ratio is dependent on the proximity of the configuration to the \(1s^2\ell\) limits in Ar\(^{15+}\) and that the ratios decrease significantly as such limits are passed.

INTRODUCTION

Single electron capture in charge exchange collisions is by now a fairly well understood process while much less is known about pick up of two electrons. Most evidence so far indicate that the pick up in many cases can be understood as a sequence of two independent events but some experimental evidence has been interpreted as indicating a correlated process. For a recent review see Reference /2/ and references therein. In order to understand which interpretation is correct and under what circumstances, knowledge about which states are being populated would be helpful. The classical models proposed, see /2/, seem to give a fairly good account of the \(n,n'\) population distribution, but much less is known about the \(\ell,\ell'\) distribution.

Doubly excited states in neutral atoms have been studied fairly extensively in recent years but less is known about the properties of this type of state in highly ionized systems.

Using translational energy gain spectroscopy it is possible to determine the ratio \(R\) between the radiative and the total decay rate for the doubly excited states /3/. We have considered whether this information can be used to decide which states are populated in pick-up to configurations of the type \(1s^2n\ell n'\ell'\) in charge exchange collisions involving Ar\(^{16+}\) and neutral rare gases. For this purpose calculations have been carried out of radiative and non-radiative decay rates averaged over the states of a \(n\ell n'\ell'\) configuration \((n \approx n' \approx 8)\) for a number of \(\ell,\ell'\) values in Ar\(^{14+}\). The results show that the
distance from a particular configuration to the next lower limit is an important factor in determining the ratio \( R(n_l,n'l') \). In neutral atoms this distance is also important but all the configurations under consideration can in this case usually decay to one and the same limit while this is not the case for large \( n,n' \) values in highly ionized atoms. With increasing energy of the bound state a new continuum might become available and boost the non-radiative decay rate. That the non-radiative decay of doubly excited states is preferentially to the nearest continuum has been observed experimentally, see Niehaus /2/ and references therein, and is due to the better overlap between low-energy continuum wavefunctions and the bound orbitals.

**METHOD**

The calculations were carried out using the suite of programs described by Cowan /4/. The approximate-relativistic HFR method introduced by Cowan and Griffin /5/ was used in a single configuration approximation in which the radiative decay of the \( n_n'i' \) configuration to all lower lying \( n''(l\pm1)n'l' \) and \( nmn''(l''\pm1) \) configurations were considered as well as the autoionization to the 4s, 5s and 6s limits. No scaling of the radial integrals was used. The total decay rates were calculated assuming the configuration to be statistically populated and the ratio \( R(n_l,n'l') \) between the radiative decay rates and the total ones evaluated. The configurations considered were the \( nsn'i, ndn'i \) and \( ndn'k \) configurations for \( n,n'=6,7,8 \) and 9. This choice of configurations is suggested by the two step models in which the pick up is understood as two independent events which limits the \( n,n' \) values to \( n \lesssim n' \).

One difficulty in the calculations is that it is known that doubly excited states of the type \( nfn'i' \) in the He sequence are strongly correlated and that the individual states cannot be described by single-configuration calculations. However, since we are averaging over all states of a particular configuration, the effect of configuration interaction is probably not severe although it can be expected to reduce the spread in \( R(n_l,n'l') \) as a function of \( l,l' \).

**RESULTS**

The position of the \( n,n'=6,7; 7,7; 7,8; 7,9; 8,8; 8,9 \) and 9,9 configurations relative to the 1s\(^2\)4\(l\); 5\(l\); 6\(l\) and 7\(l\) limits are shown in Figure 1.

It can be seen that the \( n,n'=7,6 \) configurations can autoionize only to the 4\(l\) continua while \( n,n'=7,7; 7,8; 7,9 \) and 8,8 can decay also to 5\(l\) continua. In fact \( n,n'=7,7 \) is very close to the 5\(l\) limits. The \( n,n'=8,9 \) and 9,9 configurations can in addition decay to 6\(l\) continua. This situation is important for an understanding of the variation in \( R \) as a function of \( n_l,n'l' \). The calculated \( R \) values are all considerably smaller than 1 and show a decrease when a configuration is located just above a limit as for example \( 7l7l' \) and \( 8l9l' \). The calculated values of \( R \) are given in Table I.
Table I.
Calculated values of the ratio $R(n_l,n_{qi}')$ between the radiative and the total decay rates for $1s^2n_l,n_{qi}'$ configurations in Ar $^{14+}$ averaged over all states of the $n_l,n_{qi}'$ configurations in a single configuration approximation using HFR wavefunctions

<table>
<thead>
<tr>
<th>Configuration</th>
<th>$nsn'i$</th>
<th>$rdn'i$</th>
<th>$ndn'k$</th>
</tr>
</thead>
<tbody>
<tr>
<td>6,7</td>
<td>0.092</td>
<td>0.16</td>
<td></td>
</tr>
<tr>
<td>7,7</td>
<td>0.009</td>
<td>0.017</td>
<td></td>
</tr>
<tr>
<td>7,8</td>
<td>0.016</td>
<td>0.032</td>
<td>0.080</td>
</tr>
<tr>
<td>7,9</td>
<td>0.025</td>
<td>0.051</td>
<td>0.13</td>
</tr>
<tr>
<td>8,8</td>
<td>0.027</td>
<td>0.044</td>
<td>0.12</td>
</tr>
<tr>
<td>9,8*</td>
<td>$\leq 0.012$</td>
<td>$\leq 0.021$</td>
<td>$\leq 0.023$</td>
</tr>
<tr>
<td>9,9*</td>
<td>$\leq 0.017$</td>
<td>$\leq 0.033$</td>
<td>$\leq 0.045$</td>
</tr>
</tbody>
</table>

* autoionization to 6hei has been neglected.

The decrease in $R$ at $8\ell 9\ell'$ is much smaller than at $7\ell 7\ell'$. This is because the distance between limits decrease with increasing $n$. Thus the difference in the energy of the free electron between two consecutive limits $n$ and $n+1$ decreases with $n$ and the "boost" in autoionization consequently decreases. The difference in autoionization to $n=5$ compared to $n=4$ limits is typically a factor 25 while the difference between $n=6$ and $n=5$ is about 10 times smaller. The experimental observation that autoionization is to the nearest limit only /2/ is therefore likely to be less strictly true at high values of $n$. 
There is a dependence on $g$ and $g'$ also as it can be seen that $R$ increases with increasing $g, g'$. This is expected since autoionization has a dependence on $1/\epsilon^k$ where $k$ has been found to be larger than 5 for some types of decays /6/. Such a strong dependence is not observed for the $R$ values but the variation seems significant. For a configuration like $8d8k$, $R$ is calculated to be 0.12. It is interesting that a value of 0.16 has been measured by Hvelplund /3/ for double capture in $Xe^{15+}$ on $Ar$ where similar $n, n'$ values are expected to be populated. If it is possible to make any conclusions from this value obtained for a different system it would be that the electrons appear to be picked up preferentially with a large $g$ value. In reality it can be expected that a considerable number of levels from different configurations are populated and the experimental values can be expected to be a complicated average over different configurations. From the numbers shown in Table I it is probably not realistic to expect that it is possible to use experimental values of $R$ to identify the states which are populated in double capture. For that the variation between the calculated $R$ values appears to be too small. Even though only a few different types of configurations have been considered it seems unlikely that a much larger variation exists. However, it might be possible to observe the discontinuities in $R$ when the populated levels cross a ionization limit. Similarly, in single-electron pick up the electron is expected to be picked up in states with larger values of $g$ when the relative velocity of the collision partners increases /7,8/. If two-electron pick-up is a combination of two single pick-ups it might be possible, judging from the results in Table I to observe a velocity dependence of $R$.

Finally, it should be mentioned that the same process is of interest in the case of neutralization of highly ionized atoms at surfaces, see for example the review by F.W. Meyer in these proceedings /9/. The main difference is that the initial states in this type of experiment are expected to have very low angular momentum.

ACKNOWLEDGEMENT

I wish to thank P. Hvelplund for drawing my attention to this problem and for stimulating discussions.

REFERENCES

/6/ see ref. 4 page 557.


/9/ Meyer, F.W., Havener, C.C., Reed, K.J., Snowdon, K.J. and Zehner, D.M., these proceedings.