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LETTER TO THE EDITOR

Electron impact excitation of autoionising levels in heavy alkali atoms

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Abstract. Electron excitation cross sections for six autoionising configurations of K, Rb and Cs are calculated within the Born approximation for incident electron energies up to 600 eV. Semi-empirical atomic wavefunctions are used. Values of cross sections obtained are smaller than in previous Born calculations. Cross sections for excitation of d states significantly exceed cross sections for excitation of s and p states.

Excitation of the inner n_0p-shell electrons ($n_0 = 3, 4, 5$ for K, Rb, Cs) leads to autoionising levels observed in electron impact ionisation (Nygaard 1975, Ross *et al* 1975). Theoretical calculations of cross sections for a number of autoionising levels within the Born and distorted-wave approximations using the partial-wave method have been performed by Liepinsh and Rabik (1972) and Rabik (1975). Cross sections for the lowest autoionising level $(n_0 + 1)$s within the Born and other approximations without partial-wave expansions were calculated by Tiwary and Rai (1975). Their results are approximately ten times larger than those by Liepinsh and Rabik.

We have calculated excitation cross sections for the first six autoionising configurations within the Born approximation without a partial-wave expansion. The Born cross section for the transition

$$(n_0\mathrm{p})^6(n_0 + 1)\mathrm{s} \rightarrow (n_0\mathrm{p})^5(n_0 + 1)\mathrm{s}\, nl \tag{1}$$

in atomic units is (Vainshtein *et al* 1973)

$$\sigma_{nl} = 24\pi k_0^{-2} c_{nl} \sum_t b_{lt} \int_{q_1}^{q_2} (R_{nlt}(q))^2 q^{-3}\, \mathrm{d}q \tag{2}$$

$k_0^2 = 2E$, E is the energy of the incident electron. $c_{nl} = 1$ if $nl = (n_0 + 1)$s and $c_{nl} = 2$ in other cases.

$$b_{lt} = (2l + 1)(2t + 1)\begin{pmatrix} 1 & l & t \\ 0 & 0 & 0 \end{pmatrix}^2 \tag{3}$$

$\left(\begin{smallmatrix} 1 & l & t \\ 0 & 0 & 0 \end{smallmatrix}\right)$ is a 3-j symbol. The non-zero values of b_{lt} for $l \leqslant 2$ are $b_{01} = b_{10} = 1$, $b_{12} = b_{21} = 2$, $b_{23} = 3$.

$$R_{nlt}(q) = \int_0^\infty P_{n_0 p}(r)(j_t(qr) - \delta_{t0})P_{nl}(r)\, \mathrm{d}r \tag{4}$$

$j_t(qr)$ is a spherical Bessel function and $P_{nl}(r)$ is the atomic radial wavefunction.

$$q_1 = k_0 - k_1 \qquad q_2 = k_0 + k_1 \tag{5}$$

$$k_1^2 = 2(E - D_{nl}) \qquad D_{nl} = E_{nl} - E_{n_0p} - \Delta. \tag{6}$$

E_{nl} is the binding energy of state nl and D_{nl} is the excitation threshold. The quantity Δ accounts for the shift of energy for electrons excited from the inner shell. The final energy E_{nl} ($n > n_0$) was taken as equal to the experimental value averaged over the total angular momentum. The initial energy E_{n_0p} was found as a sum of the neutral-atom experimental ionisation energy and the averaged experimental excitation energy of the ion. The shift Δ was chosen so that the threshold for the transition $n_0p \rightarrow (n_0 + 1)s$ was equal to the experimental value. All experimental values were taken from Moore's tables (Moore 1958). Some atomic constants used by us are given in table 1.

Table 1. Atomic constants.

	E_{n_0p}(eV)	$D_{(n_0+1)s}$(eV)	Δ(eV)	d	H
K	−24·66	18·80	1·52	1·006	3·197
Rb	−21·16	15·59	1·39	0·744	3·120
Cs	−17·86	12·71	1·25	1·022	5·040

Atomic wavefunctions were found by numerical integration as eigenfunctions of the radial equation

$$\left(\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} - 2V_{nl}(r) + 2E_{nl}\right)P_{nl}(r) = 0. \tag{7}$$

The analytic expression of Green *et al* (1969) was used for the potential

$$V_{nl}(r) = -\frac{1}{r}\left(\frac{Z-1}{H[\exp(r/d) - 1] + 1} + 1\right). \tag{8}$$

Z is the atomic number, d and H are parameters. Green *et al* have given values of the parameter d which provide an approximation to the Hartree–Fock potential if

$$H = d(Z - 1)^{0.4}. \tag{9}$$

These parameters are given in table 1.

In our calculations of wavefunctions we introduced a semi-empirical modification. Parameter H remained unchanged, while the parameter d was found for each nl separately so that the eigenvalue of equation (7) agreed with the experimental value of E_{nl}. Shift Δ in this case was not taken into account.

Table 2 contains the parameter d and the excitation cross sections for six autoionising configurations of K, Rb and Cs. Cross sections for the lowest autoionising level were also calculated using simple Slater-type wavefunctions (Clementi and Raimondi 1963, Clementi *et al* 1967). In table 2 these cases are indicated by daggers. It is seen that the use of Slater-type wavefunctions increases the cross section for K and reduces it for Cs.

Slater-type wavefunctions were also used by Tiwary and Rai (1975). Cross sections obtained by us for this case are similar in shape though 23–25 times smaller in

Table 2. Potential parameters and excitation cross sections (cross sections in units of πa_0^2).

	nl	*d* \ *E*(eV)	30	40	50	70	100	200	400	600
K	3p	0·985								
	4s	0·913	0·020	0·028	0·032	0·033	0·032	0·024	0·017	0·013
	4s	†	0·058	0·066	0·066	0·062	0·055	0·038	0·024	0·018
	5s	0·915	0·005	0·008	0·009	0·010	0·010	0·008	0·005	0·004
	4p	0·919	0·056	0·059	0·055	0·045	0·034	0·019	0·010	0·007
	5p	0·917	0·014	0·016	0·015	0·012	0·010	0·005	0·003	0·002
	3d	0·902	0·204	0·248	0·258	0·250	0·224	0·161	0·105	0·080
	4d	0·901	0·114	0·141	0·148	0·143	0·129	0·092	0·060	0·046
Rb	4p	0·758								
	5s	0·749	0·071	0·084	0·087	0·085	0·077	0·056	0·037	0·028
	5s	†	0·090	0·094	0·092	0·084	0·073	0·050	0·031	0·024
	6s	0·744	0·017	0·022	0·024	0·024	0·022	0·017	0·011	0·008
	5p	0·741	0·115	0·106	0·094	0·074	0·055	0·030	0·015	0·010
	6p	0·737	0·028	0·027	0·024	0·019	0·014	0·008	0·004	0·003
	4d	0·755	0·932	0·995	0·980	0·900	0·780	0·535	0·341	0·256
	5d	0·751	0·395	0·430	0·427	0·394	0·342	0·236	0·150	0·113
Cs	5p	1·003								
	6s	0·990	0·149	0·163	0·164	0·155	0·138	0·100	0·064	0·049
	6s	†	0·135	0·135	0·129	0·115	0·097	0·065	0·041	0·031
	7s	0·990	0·036	0·042	0·044	0·043	0·039	0·028	0·019	0·014
	6p	0·981	0·209	0·184	0·160	0·125	0·093	0·050	0·026	0·017
	7p	0·978	0·051	0·046	0·041	0·032	0·024	0·013	0·007	0·004
	5d	0·968	3·410	3·450	3·320	2·970	2·540	1·710	1·080	0·810
	6d	0·967	0·780	0·798	0·772	0·695	0·594	0·401	0·253	0·190

magnitude. We use average threshold values while Tiwary and Rai used the lowest value. Using the lowest threshold value we obtained results nearly 24 times smaller than those obtained by Tiwary and Rai.

Our results are several times smaller than the Born approximation results by Liepinsh and Rabik (1972) and Rabik (1975). This discrepancy may be caused by use of different atomic wavefunctions.

An interesting feature is that the cross sections for excitation of d states significantly exceed the other cross sections. This can be explained by the behaviour of the d-state wavefunctions which are located relatively near to the n_0p wavefunction.

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