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The lifetime of Mg^-: $3p^3\ ^4S^o$

ABSTRACT

The decay of $Be^-\ 2p^3\ ^4S^o$ was observed by Gaardsted and Andersen (1989) and the decay of $Mg^-\ 3p^3\ ^4S^o$ is under investigation by Andersen (1989). Accurate theoretical data can help with the detection of this process. Preliminary analysis of the experimental data disagreed for the lifetime with calculations by Beck, 1984. Beck (1989) has since improved on his earlier work. This paper presents an entirely independent approach to a lifetime calculation. The results are in excellent agreement with those of Beck, 1989.

THE CALCULATION

The close coupling approximation is used on two different target models. In both models atomic orbitals are optimised for the weighted sum of the energies of the lowest ten terms of magnesium. The MCHF program by Froese-Fischer,1978 with modifications by Trefftz, 1988 is used. Model A includes configurations $3s^2$,3s4s,3s5s,3s3d,3s4d,$3p^2$,$3d^2$,$4s^2$,3p4p,3d4d, 3s3p,3s4p,3p3d, and 3p4s. This model gives poor energies for the higher terms of odd parity, see table 1. Model B uses in addition configurations $2p^5$3s3p3d,$2p^5$$3s^2$5s,$4p^2$,3p4d. This model gives a better representation of the higher terms. Tne target models were developed for a scattering calculation, where one aims for a reasonably good representation of *all* the lowest 'closely coupled' terms. Only few of these terms contribute to scattering channels for compound states ^4P and $^4S^o$ and these are listed in table 1. The compound system $Mg+e^-$ is described by the wavefunction

$$\Psi^{SL\pi} = A\Sigma\phi_i F_i + \Sigma c_j \Phi_j \qquad (1)$$

Where A is an antisymmetrisation operator, ϕ and F are vector coupled functions for target and added electron states, and the Φ describe compound states using only target orbitals. Allowing the radial part of F and the configuration mixing coefficients c to vary freely one obtains a set of coupled integro-differential equations for each $SL\pi$. The program COLALG by Eissner, 1972 is used for the algebraic part and the program IMPACT by Crees *et al.*, 1978 for the radial part of the solutions. With these wavefunctions and the coefficients for radiative transitions produced by the program RADALG (Jones, 1974, Eissner and Jones, 1989) oscillator strengths and photoionisation cross sections can be calculated, Saraph, 1987. Spin-orbit coupling is neglected throughout.

Table 1
Term energies (in Ryd) for Mg. Experimental data are from Moore, 1949.

term	exp	model A	model B
$3s^2\ ^1S$	0.0	0.0	0.0
$3s3p\ ^3P^o$	0.1995	0.1890	0.1857
$3s4p\ ^3P^o$	0.4360	0.4714	0.4295
$3s3d\ ^3D$	0.4370	0.4315	0.4332
$3p^2\ ^3P$	0.5272	0.5111	0.5069

RESULTS

Table 2 presents electron affinities for the Mg^- bound states ^4P and $^4S^o$ obtained using the two target models. It also lists the LS-coupling results by Beck, 1989.

Table 2
Electron affinities in Rydberg for Mg^-, relative to the calculated energies of the parent terms $3s3p\ ^3P^o$ and $3p^2\ ^3P$ respectively.

term	model A	model B	Beck(LS)
$3s3p^2\ ^4P$	.0277	.0288	.0236
$3p^3\ ^4S^o$	.0395	.0347	.0394

The present electron affinities differ considerably from those of Beck, 1989. This discrepancy disappears when the wavelength is calculated. Table 3 compares wavelengths and oscillator strengths with the results by Beck 1984 and 1989. The present wavelengths are obtained from the difference of the total energies. Beck's wavelengths are obtained by subtracting the difference of the electron affinities from the inverse observed wavelength of the threshold transition. Beck includes relativistic effects and shows these to be small. It appears that the transition data are fairly stable with respect to improvements in these sophisticated calculations.

Table 3
Wavelengths and oscillator strengths for the process $3s3p^2\ ^4P - 3p^3\ ^4S^o$ (length form.)

	model A	model B	Beck, 1984	Beck, 1989
λ(Å)	2936	2909	2880	2921
f_{abs}	.310	.297	.295	.309

The agreement between the present calculation and that of Beck is very good indeed.

The term $^4S^o$ can also decay directly by radiative detachment. The cross section for this process could be calculated with the present setup. It has a broad maximum around λ=3551 Å that contributes to the decay rate by $.102*10^8\ s^{-1}$, while the decay rate to the bound state is $A=.702*10^9\ s^{-1}$. Hence, the final result for the lifetime of $3p^3\ ^4S^o$ is

$$\tau(^4S^o)=1.40\text{ns},$$

with an error estimate of 5%. The challenge is now with the experimentalists.

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