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Calculation of radiative decay rates and branching ratios in Hg^+

ABSTRACT

Pseudo-relativistic wavefunctions have been used to calculate E1, E2 and M1 radiative decay rates and branching ratios connecting levels of the three lowest lying electron configurations of Hg^+ and compared with recent accurate results obtained from fluctuations (quantum jumps) of laser-induced flourescence studies of a single ion held in an ion trap.

INTRODUCTION and METHOD

The development of ion traps, lasers and photon counting methods have allowed the determination (to within a reasonably high degree of accuracy) of experimental decay rates linking different energy levels from the observed fluctuations in laser-induced flourescence of a single transition in Hg^+ (Itano et al 1987). Referring to Fig 1 the five lowest energy levels of Hg^+ are shown. Itano et al deduced the decay rates for the allowed transition $6p\ ^2P_{1/2}$ - $6s\ ^2S_{1/2}$ and the configuration interaction (CI) induced transition $6p\ ^2P_{1/2}$ - $d^9s^2\ ^2D_{3/2}$. In addition they also determined the forbidden decay rates from the two ^2D levels back to the ground level.

Using the pseudo-relativistic Hartree-Fock model (HFR), (see eg. Cowan 1981), we first obtained single-configuration wavefunctions for the configurations: $5d^{10}6s$, $5d^96s^2$ and $5d^{10}6p$, $5d^96s6p$. These were then used to calculate the usual interaction integrals used to obtain the single and mixed-configuration structures together with the necessary transition integrals required for the appropriate E1 and E2 transitions of interest here. The mixed-configuration energy matrices were diagonalized and the resulting eigenvalues compared with the experimental data. At this stage adjustments were made to the ab initio values of the centre of gravity energies in order to give somewhat closer agreement between calculated and experimental levels. This procedure helps obtain a more realistic degree of CI mixings than that produced entirely by ab initio methods. Finally the resulting CI eigenvectors were combined with the appropriate ab initio transition integrals to calculate the E1, E2 and M1 transition rates, A, between all possible levels of interest.

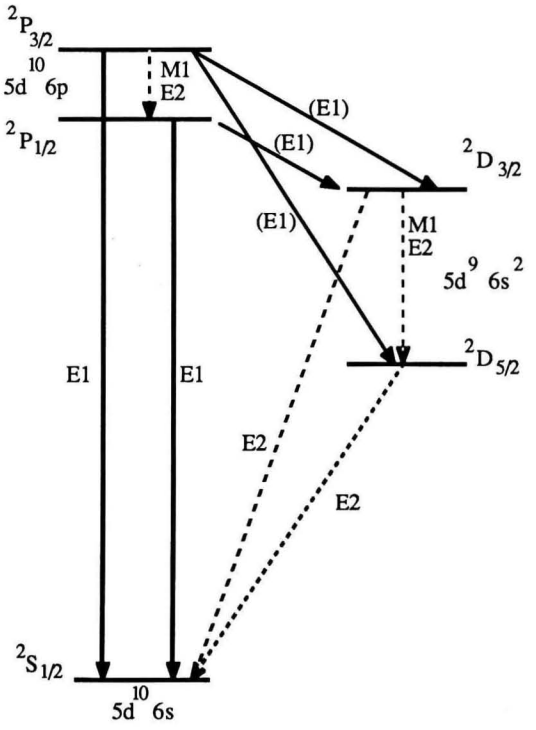

Fig. 1 Low level scheme of Hg^+

RESULTS and DISCUSSION

A selection of our results is presented in Table 1 together with the experimental data. It should be noted that in this preliminary study we have used unscaled values of the HFR transition and interaction integrals. Not unexpectedly the calculated E1 decay rate from the $^2P_{1/2}$ to the $^2S_{1/2}$ is somewhat larger than the experimental value. The weaker CI induced E1 decay to the metastable $^2D_{3/2}$ occurs due to mixing of a ^2P component of the d^9sp configuration for which we found

$5d^{10}6p\ ^2P_{1/2}> \sim 0.992\ 6p\ ^2P> + 0.127\ d^9sp\ ^2P>$ lending some of its 6p - 6s strength to the otherwise forbidden transition. Our calculated rate is is good accord with the experimental value (and an unpublished theoretical estimate quoted by Itano et al.). However, this rate is extremely sensitive to the degree of mixing as indicated

by large changes in the calculated decay rate with small changes in level positions. We also considered the effects of including additional perturbers, of both parities, which might influence this induced transition (see below).

From the results given in Table 1 we may also obtain the total radiative decay rate from $^2D_{3/2}$ being due to both an M1 and E2 contribution of comparable size ie. (55.3 + 71.9) ~ 127 s^{-1} which may be compared with the value 109 ± 5 obtained by Itano et al. Similarly we find the total radiative decay rate from the $^2D_{5/2}$ due to an E2 transition as 12.3 s^{-1} compared to (11.6 ± 0.4) found by Itano et al. Denoting the probabilities for the $^2D_{3/2}$ level to decay to the $^2S_{1/2}$ level or the $^2D_{5/2}$ level as f_1 and f_2 ($f_1 + f_1 = 1$) we obtain from the results in Table 1 f_1 ~ 0.55 whereas Itano et al found $f_1 = 0.491 \pm 0.015$. Our calculated estimate of this branching ratio could be modified to lie closer to the experimental value either by a suitably large decrease in the E2 rate from the $^2D_{5/2}$ or by some even parity mixture not yet included. We investigated the degree of modification on the E2 transition integral by re-calculating our radial wavefunctions using the usual HFR potential but augmented by an approximate correlation potential based on a free electron correlation energy, ie. the function e_c given by eqn (7.71) of Cowan (1981). Although such functions produced transition integrals of slightly smaller magnitudes the effect on the E2 rate was insufficient to account for the observed difference. We are examining the effects of including $5d^{10}6d$, $5d^9 6p^2$, $5d^8 6s 6p^2$ and $5d^8 6s^2 6p$, $5d^9 6p 6d$ but preliminary findings show that these are found to have little influence on the results obtained (with the noteable exception of the CI induced transitions) from our more restricted set of configurations. Bearing in mind the simple model used here the present calculations are gratifyingly close to the empirical values derived from a most beautifully ingenious experiment.

Table 1. Decay rates A(s^{-1}) for Hg^+

Transition				A(s^{-1}) Theory (this work)	Expt (Itano et al)
$5d^{10}6p\ ^2P_{3/2}$ -	$5d^96s^2$	$^2D_{3/2}$	(E1)	1.25×10^4	
-		$^2D_{5/2}$	(E1)	2.89×10^6	
-	$5d^{10}6p$	$^2P_{1/2}$	M1	6.85	
-		$^2P_{1/2}$	E2	0.29	
-	$5d^{10}6s$	$^2S_{1/2}$	E1	8.74×10^8	
$5d^{10}6p\ ^2P_{1/2}$ -	$5d^96s^2$	$^2D_{3/2}$	(E1)	57.7	52 ± 16
-	$5d^{10}6s$	$^2S_{1/2}$	E1	5.74×10^8	$(3.8 \pm 0.6)10^8$
$5d^96s^2\ ^2D_{3/2}$ -	$5d^96s^2$	$^2D_{5/2}$	M1	55.3 ←┐	
-		$^2D_{5/2}$	E2	0.04 127.2	109 ± 5
-	$5d^{10}6s$	$^2S_{1/2}$	E2	71.9 ←┘	
$5d^96s^2\ ^2D_{5/2}$ -	$5d^{10}6s$	$^2S_{1/2}$	E2	12.3	11.6 ± 0.4

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