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ENERGY LEVELS AND LIFETIMES OF $2p^5 3s3d$ QUARTETS IN Na I

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THE $2p^5 3s3d$ ^4L LEVELS IN NA I CAN DECAY IN THREE WAYS:

I) E1 TRANSITIONS TO $2p^5 3s3p$ LEVELS (^4L ALLOWED)

II) E1 TRANSITIONS TO $2p^6 n\ell$ ^2L (SPIN-FORBIDDEN)

III) AUTOIONIZATION TO $2p^6 k\ell$ ^2L (SPIN-FORBIDDEN)

MULTI-CONFIGURATION HARTREE-FOCK CALCULATIONS WITH BREIT-PAULI CORRECTIONS WERE PERFORMED FOR EACH MODE OF DECAY WITH SPECIAL EMPHASIS GIVEN TO THE $2p^5 3s3p$ ^4L - $2p^5 3s3d$ ^4L TRANSITIONS. SIMILAR CALCULATIONS HAD BEEN PERFORMED BY HOLMGREN ET AL. (1985) USING COWAN'S CODE, RCN/RCG.

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Accurate spin-orbit mixing is crucial in this problem. Thus any radial basis must well represent both doublets and quartets. As a first step we explored the term dependence of the orbitals. Fig. 1 shows the variation in the 3d orbitals for the three couplings

$$(^3P)\ ^4L,\ (^3P)\ ^2L,\ \text{and}\ (^1P)\ ^2L$$

The orbitals were relatively insensitive to the final L-value. With term dependence taken into account, term mixing was somewhat reduced (see Table 1). At the same time, the fine-structure splitting agreed well with experiment. (see Table 2).

A reduction in doublet-quartet mixing should result in a reduction of the autoionization rate for the doublets. This was found not to be the case. Comparison with results of the Cowan code for $2p^5 3s3p$ (Harris et al. 1984) showed that orthogonality of orbitals and how non-orthogonality was treated, greatly influenced the computed autoionization rate. Table 3 compares values obtained in different ways.

Finally, in Table 4, we compare lifetimes derived from the two approaches to values determined from experiment. The $^4P_{5/2}$ level is metastable against autoionization. Though the present lifetime is in better agreement with experiment, it is still almost a factor two longer. The $(^3P)3d\ ^4F_{9/2}$ level is also mestastable and the present lifetime is in much better (though not great) agreement with experiment. The $(^3P)3d\ ^4P_{1/2}$ level is an example where a larger autoionization rate has resulted in better agreement with experiment.

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TABLE 1 COMPARISON OF WAVEFUNCTION EXPANSIONS FOR $(^3P)3d\ ^4F_{5/2}$.

MCHF + BP

$$0.76\ (^3P)3d\ ^4F - 0.55\ (^3P)3d\ ^4P + 0.22\ (^3P)3d\ ^4D - 0.18\ (^1P)3d\ ^2D$$

RCN/RCG

$$0.73\ (^3P)3d\ ^4F - 0.58\ (^3P)3d\ ^4P - 0.26\ (^1P)3d\ ^2D$$

Table 2   Energy levels (in cm^{-1}) for $(^3P)3p$ quartets relative to $^4S_{3/2}$

Term	J	Theory	Obs.[a]	Diff
^4D	7/2	2726	2841	115
	5/2	3084	3187	103
	3/2	3434	3536	102
	1/2	3726	3830	104
^4P	5/2	4795	4768	-27
	3/2	5179	5152	-27
	1/2	5381		

[a]Holmgren et al. (1985)

TABLE 3 EFFECT OF ORTHOGONALITY ASSUMPTIONS ON $2p^5 3s3p$ $^4P_{1/2}$ AUTOIONIZATION RATE A, IN Na I, WHERE

$$A = 1.2988 \times 10^{17} \langle 2p^5 3s3p | H-E | 2p^6 \kappa s \rangle^2$$

	A
1. RCN/RCG	
A) 1s, 2s, 2p DIFFERENT FOR THE TWO STATES	
B) NO ORBITALS ORTHOGONAL	
C) MATRIX ELEMENT EVALUATED	
I) H-E REPLACED BY V	
II) KS ASSUMED ORTHOGONAL TO 3s	10.1×10^{10}
2. MCHF + BP	
A) 1s, 2s, 2p THE SAME FOR BOTH STATES	
B) 3s, KS BOTH ORTHOGONAL TO 1s AND 2s	
C) MATRIX ELEMENT EVALUATED	
I) H-E, WITH OVERLAPS	$102. \times 10^{10}$
II) KS ASSUMED ORTHOGONAL TO 3s	22.7×10^{10}
III) KS REQUIRED TO BE ORTHOGONAL TO 3s	15.3×10^{10}

TABLE 4 LIFETIMES OF SOME $2p^53s$ NI QUARTETS

TERM	J	PRESENT	OTHER[A]	EXPERIMENT[B]
4S	$^4P_{5/2}$	8.3	10.9	4.4 ± 0.4*
3D	$^4P_{1/2}$	2.4	5.8	2.95 ± 0.2
	$^4P_{3/2}$	4.6	2.8	4.10 ± 0.4
	$^4P_{5/2}$	4.7	6.1	3.34 ± 0.2
3D	$^4F_{9/2}$	5.1	6.1	4.38 ± 0.2*
	$^4F_{7/2}$	1.4	2.9	0.94 ± 0.15
	$^4F_{5/2}$	0.2	0.18	0.40 ± 0.20

*THESE LEVELS ARE METASTABLE AGAINST AUTOIONIZATION.

[A]HOLMGREN ET AL. (1985).

[B]ENGSTROM ET AL. (1985).

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