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FINE STRUCTURE TRANSITION CROSS SECTIONS FOR SEVERAL ALKALI + RARE GAS SYSTEMS

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The energy dependence, $E_{cm} \leq 0.2$ eV. of the inelastic total cross sections for the $^2P_{1/2} \rightarrow {}^2P_{3/2}$ fine structure transition of the lowest excited states of the alkali are calculated for the following systems : Na, K, Rb + He, Ne, Ar and Cs + He. Encouraging agreement between theory and experiment is obtained.

In recent papers by Reid and Dalgarno /1/ and Reid /2/, these authors have cleverly formulated a quantum mechanical theory for fine structure transitions of the lowest ^2P states of an alkali atom on collision with a rare gas atom. The method is an extension of the Arthurs and Dalgarno /3/ treatment for rotational excitation of a rigid rotor. In a comprehensive paper, Reid /2/ has displayed this method in the calculation of both the total and differential inelastic cross sections for fine structure transitions between the $3^2P_{3/2}$ and $3^2P_{1/2}$ states of Na on collision with He. The method is equally applicable to other alkali + rare gas systems and possesses several advantages over classical trajectory methods that are also currently in use /4/, /5/. Some of the advantages are that there is no problem with choosing an appropriate average trajectory nor any difficulty with calculating the cross section near the energy threshold (important for the heavier alkalis). Also, the effects of quasi-bound states

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(important for the heavier rare gases) are intrinsically included in the quantum calculations.

In this paper, we have utilized the method of Reid /2/ and the pseudo-potential calculations of Baylis /6/ to calculate the intra-multiplet mixing total cross sections for a range of alkalis and rare gases. Also, Maxwellian averaged cross sections are calculated so that we may compare the results to existing experimental data.

A schematic diagram of the alkali + rare gas interaction potentials is shown in Fig. 1. The total inelastic cross sections are calculated for transfer from the $^2P_{1/2}$ state of the alkali to its $^2P_{3/2}$ state. The calculations for the Na, K, Rb + He, Ne, Ar and Cs + He systems are presented in Figs. 2-4. In order to compare with experiment, the cross sections shown were Maxwellian averaged. The resulting cross section values are given in Table I. The calculations not only show the correct trend of the cross section with various rare gases for a given alkali, but are in very reasonnable agreement with experiment. Depicted clearly in the threshold dependence, is the reason why Ne + K or Rb has a smaller thermal averaged cross section than either He or Ar. Physically, this effect is caused by less attractive interaction potentials for Ne with K or Rb than for either He or Ar. Also reproduced, are the orders of magnitude change in the cross sections as we proceed to the heavier alkalis. In fact, for the heavier alkalis the agreement between theory and experiment is striking considering the magnitudes of the cross sections.

At this time, the calculations were only extended to the heavier rare gases, Kr and Xe for collisions with Na, because of the expensive necessity of needing a very fine energy grid to accurately obtain these cross sections. In these cases, the $A^2\Pi_{1/2}$ potential well is very deep, so we are plagued with quasi-bound states for thermal energy collisions that give rise to very irregular structure on the cross sections. For this reason, the Na + Ar cross sections shown in Fig. 2 are displayed by dashed lines, since even though the energy

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grid was 0.001 eV, it is not sufficiently fine to accurately depict all the structure that is present. For Na + Kr and Xe, we have calculated the Maxwellian averaged cross sections and find Q (400°K, Na Kr) = 1.3×10^{-14} cm^2 and Q (400°K, Na Xe) = 1.2×10^{-14} cm^2. These values may be compared to the experimental values of Pitre and Krause /7/ who find 8.5×10^{-15} cm^2 and 9.0×10^{-15} cm^2, and to the values of Schneider /8/ who finds 9.4×10^{-15} cm^2 and 9.9×10^{-15} cm^2, respectively. Because the cross sections have extreme oscillations due to quasi-bound levels, we prefer to only report the above figures with the reservation that the calculated values are accurate to ca. 10%.

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TABLE I : CALCULATED $^2P_{3/2} \leftarrow {}^2P_{1/2}$ FINE STRUCTURE TRANSITION CROSS SECTIONS COMPARED TO EXPERIMENT.

System	E(cm^{-1})	Reference	T(°K)	He-Q(cm^2)	Ne-Q(cm^2)	Ar-Q(cm^2)
Na	17	This work	400	7.5(-15)[a]	8.6(-15)	1.05(-14)
		Réf. 7	397	8.6(-15)	6.7(-15)	1.10(-14)
		Réf. 8	400	8.9(-15)	7.9(-15)	1.16(-14)
K	58	This work	400	3.3(-15)	7.3(-16)	1.3(-15)
		Réf. 9	368	6.0(-15)	1.4(-15)	3.7(-15)
Rb	238	This work	400	7.2(-18)	7.0(-20)	1.6(-19)
		Réf. 10	400	7.7(-18)	2.2(-19)	7.5(-20)
		Réf. 11	340	7.6(-18)	1.7(-19)	1.0(-19)
Cs	554	This work	400	1.0(-20)	-	-
		Réf. 10	400	1.3(-20)		
		Réf. 12	311	5.7(-21)		

a. 7.5 (-15) means 7.5×10^{-15}

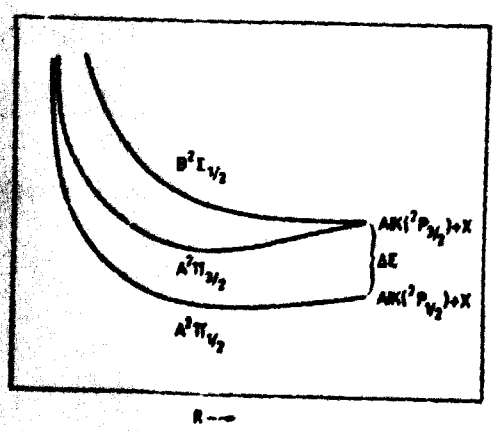

Figure 1

Schematic diagram of the alkali + rare gas interaction potentials.

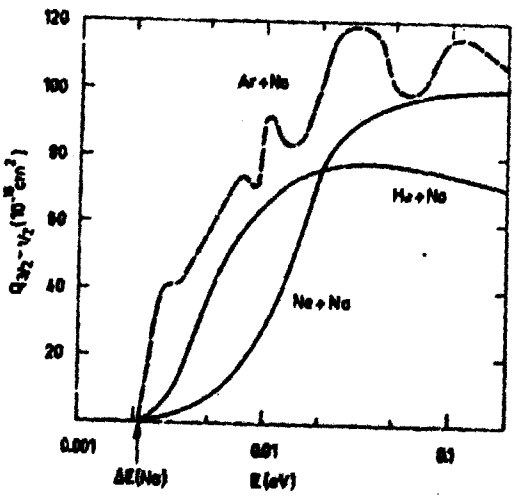

Figure 2

Na ($3\,^2P_{3/2} \leftarrow 3\,^2P_{1/2}$) cross sections for collisions with He, Ne, and Ar.

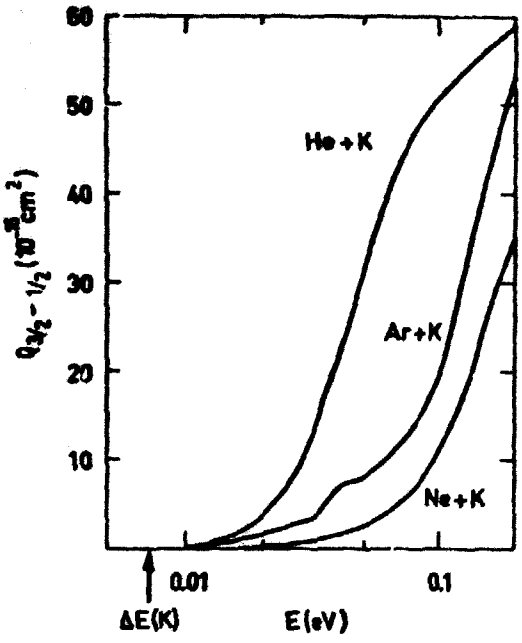

Figure 3

$K(4\,^2P_{3/2} \leftarrow 4\,^2P_{1/2})$ cross sections for collisions with He, Ne, and Ar.

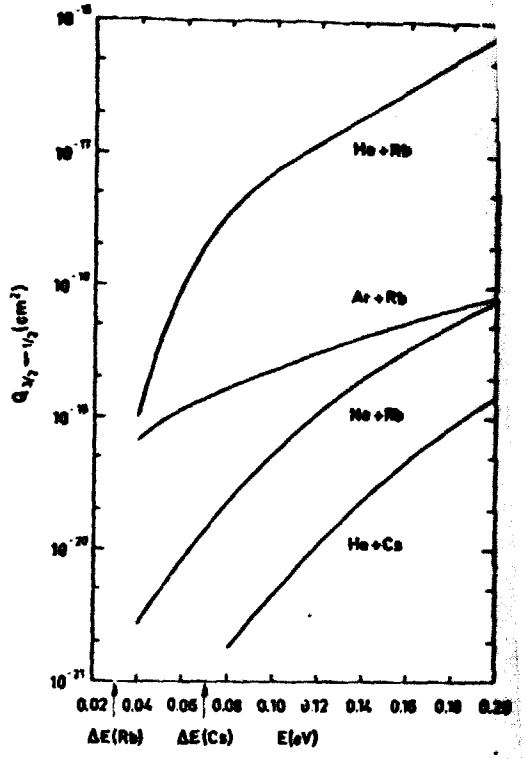

Figure 4

$Rb\,(5\,^2P_{3/2} \leftarrow 5\,^2P_{1/2})$ cross sections for collisions with He, Ne, and Ar; and the $Cs\,(6\,^2P_{3/2} \leftarrow 6\,^2P_{1/2})$ + He cross section.