

Inclusive probabilities for the scattering system 16 MeV-S¹⁶⁺ on Ar

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Abstract

We performed *ab initio* calculations of many particle inclusive probabilities for the scattering system 16 MeV-S¹⁶⁺ on Ar. The solution of the time-dependent DIRAC-FOCK-SLATER-equation is achieved via a set of coupled-channel equations with energy eigenvalues and matrix elements which are given by static SCF molecular many electron calculations.

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During the last few years we developed a fully *ab initio* DIRAC-FOCK-SLATER (DFS) molecular code [1] which is able to provide energy eigenvalues and matrix elements between single particle levels. Using this input we are now able to perform coupled channel calculations. Knowing the transition amplitudes between the channels one is able to calculate inclusive probabilities [2, 3] for many electron transfer and excitation in many electron collision systems. Such a calculation is equivalent to the solution of the time dependent Dirac-Slater equation of the scattering problem with an adiabatic interaction potential. As a first example we have chosen the system 16 MeV-S¹⁶⁺ on Ar [4]. The experiment was carried out to answer the following questions: How large is the probability of finding:

1. One electron in Ar 1s and one electron in S 1s? (P_{SA})
2. Two electrons in Ar 1s? (P_{SS})
3. Two electrons in S 1s? (P_{AA})

We performed a large number of selfconsistent static DFS calculations of the quasi molecular system S¹⁶⁺ - Ar at many internuclear distances to obtain the adiabatic energy eigenvalues as well as the d/dR and d/dw coupling-matrix elements with an occupation according to the asymptotic occupation of the separated atoms in the incoming channel. This leads to the correlation diagram presented in Fig. 1. Due to the high degree of ionization the lowest level of this system for large internuclear distances is the 1s level of S although its Z value is smaller than the one for Ar.

In the actual coupled-channel calculation we included the 20 lowest relativistic channels (8 non relativistic

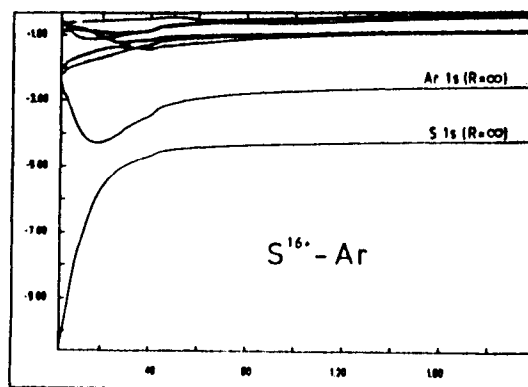


Figure 1: Correlation diagram : S¹⁶⁺-Ar

channels) and calculated the amplitudes of the four lowest molecular levels (each doubly degenerate) which form the separated Ar 1s and S 1s levels after the collision. To evaluate the many particle probabilities we express the inclusive probabilities P_{SS} , P_{AA} and P_{SA} in terms of one electron amplitudes. The index S, resp. A, denotes a measured hole in the 1s shell of the Sulfur, resp. Argon. The 16 combinations to distribute zero to four electrons in the 1s shells of Sulfur and Argon are given in Tab. 1. The probabilities of each of these combinations were calculated exclusive within the four lowest channels but inclusive with respect to the other channels. To get P_{SS} , P_{AA} and P_{SA} we sum up the probabilities of those combinations that contribute to the many particle probabilities considered according to the right side of Tab. 1. Probabilities of those combinations contributing to more than one many particle probability are distributed equally among them.

Figs. 2 and 3 show the inclusive probabilities P_{AA} , P_{SS} and P_{SA} in comparison with the results of [4] i.e. P(b)-curves for the questions 1 to 3. The inclusive (four particle exclusive) probabilities will be published soon [5].

Occupation				P _{SA}	P _{AA}	P _{SS}
S 1s+	S 1s-	Ar 1s+	Ar 1s-			
o	o	o	o	◇	◇	◇
●	o	o	o	◇	◇	
o	●	o	o	◇	◇	
o	o	●	o	◇		◇
o	o	o	●	◇		◇
o	o	●	●			◇
o	●	●	o	◇		
●	●	o	o		◇	
●	o	o	●	◇		
o	●	o	o	◇		
●	o	●	o	◇		
●	●	●	o			
o	●	●	●			
●	o	o	●			
●	●	o	●			
●	●	●	●			

Table 1: The 16 possible ways of putting 0, 1, 2, 3, or 4 electrons into 4 levels and contribution to the inclusive probabilities. ●: occupied; o: unoccupied

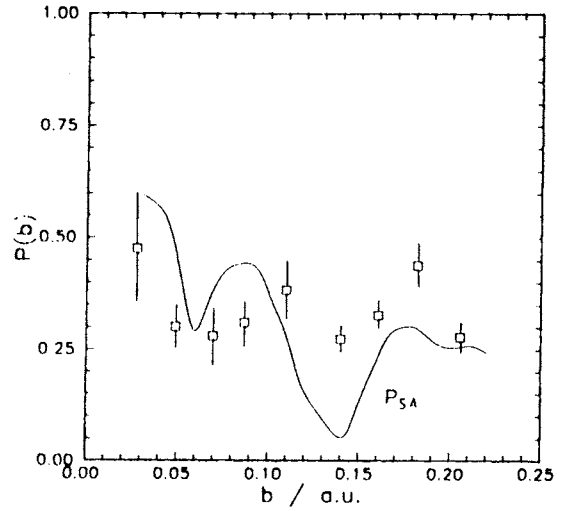


Figure 3: P_{SA}

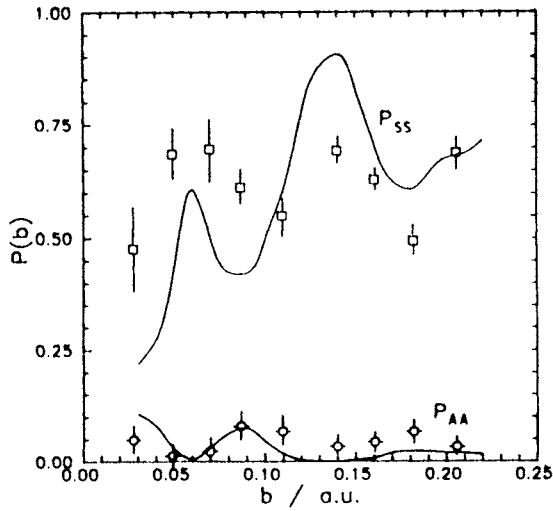


Figure 2: P_{AA} and P_{SS}

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