Propensity rules for magnetic-substate distributions for electron capture from excited states of atoms by multiply charged ions

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The propensity rules for populating magnetic substates in electron-capture processes from excited target atoms are examined theoretically using the close-coupling expansion method with two-center atomic orbitals. It is shown that if the quantization axis is chosen to be perpendicular to the scattering plane, the dominant magnetic substate populated for each final nl state is $m=-l$, irrespective of the magnetic quantum number of the initial state. Electron-capture processes from $2s$ and oriented $2p$ states of hydrogen atoms in collisions with He^{2+} and Li^{3+} are examined.

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I. INTRODUCTION

In a recent paper, Lundsgaard and Lin [1] examined the magnetic-substate distributions of excited states populated by electron-capture processes in collisions between multiply charged ions with atoms. It was observed that if the quantization axis is chosen to be perpendicular to the scattering plane, the probability for electron capture to the $m=-l$ component is largest within the degenerate magnetic substates. This propensity rule implies that the electron which is captured stays mostly near the collision plane ($|m|=l$) and that its sense of rotation is identical to that of the internuclear axis (negative m). The calculations have been carried out and tested for $C^{6+}+H(1s)$, and the propensity rule has been shown to be valid for transitions at large impact parameters and for projectiles with velocities near the target electron's orbital velocity.

The purpose of this article is to examine the dependence of the electron-capture cross section on the *orientation,* or the magnetic quantum number, of the initial state of the target. Such an experiment has been carried out recently be measuring the differential electron-capture cross section for collisions between protons and oriented $Na(3p)$ atoms at a number of energies [2]. Instead of comparing calculations and experiments for a specific system, our goal in this paper is to discover some possible systematic trends, or propensity rules, for the dependence of electron-capture probabilities on the initial orientation of the target atom. We have chosen different orientations of $H(2p)$ as the target excited states. Because of the strong coupling between $H(2s)$ and $H(2p)$, we also examine electron-capture probabilities from $H(2s)$.

For heavy-particle collisions, the angular scattering of the projectile is very small, and there are very few experimental studies of the dependence of electron-capture cross sections on the orientation of the target atom. On the other hand, a number of experiments have examined the dependence of electron-capture cross sections on the *alignment* of the excited target atom [3–5], where differential measurement is not required. For $p+Na(3p)$ collisions, it has been observed [3] that electron-capture cross section is larger if the target atom is aligned parallel to the incident-beam direction than if it is aligned perpendicular to the beam. However, the opposite is true for $He^{2+}+Na(3p)$ collisions [4]. In a recent theoretical study, Esry *et al.* [6] examined the effect of alignment of $H(2p)$ in $H^{+}+H(2p)$ and $He^{2+}+H(2p)$ collisions. They found that in both cases electron-capture cross sections from $H(2p)$ are larger if $H(2p)$ is aligned parallel to the beam than if it is aligned perpendicular to the beam. Thus it appears that there is no general rule for the dependence of electron-capture cross sections on the alignment of the initial state.

An aligned initial state has anisotropic electron-density distributions. For each electron-capture event, it is well known that the momentum distribution of the initial state is the dominant factor in determining electron-capture cross sections at high velocities. Since each capture event is also accompanied by a change in the angular momentum of the electron, we speculate that the initial *orientation* of the target electron is more important in determining the relative magnitude of electron-capture cross sections. Thus our goal in this paper is to examine whether electron-capture probabilities favor specific orientations of the initial states. In addition, we also examine electron-capture processes from $H(2s)$.

Section II describes briefly the computational methods and the coordinate system used. The results are presented and analyzed in Sec. III for Li^{3+} and He^{2+} colliding with $H(2s)$ and $H(2p)$ states. A brief summary and discussion is given in Sec. IV. Atomic units are used throughout this paper unless otherwise noted.

II. THEORETICAL METHODS

We examine electron-capture probabilities and cross sections based on the close-coupling method using atomic orbitals on both collision centers [7]. The method has

been shown to be valid for collisions with atoms in the ground state in the energy range of interest in this paper. In the present calculation, each atomic orbital is expanded in terms of Gaussian-type orbitals (GTO's) [8]. The number of GTO's used to diagonalize the atomic Hamiltonian on each center is 40, 30, 25, and 25 for $l=0$, 1, 2, and 3, respectively, and the diagonalization reproduces the spectrum of all the $n \leq 4$ excited states on each center. The use of Gaussian orbitals allows us to evaluate all single-center matrix elements analytically and all two-center matrix elements in terms of incomplete Γ functions [8]. It is noted that all the matrix elements are evaluated using Cartesian coordinates so that the computation of matrix elements does not depend on the axis of quantization. In the present work, the quantization axis was chosen to be perpendicular to the scattering plane.

For the purpose of discussion, we choose the natural coordinate system [9] as shown in Fig. 1. The collision plane is the plane of the paper with the x axis in the direction of the incident beam. The y axis is chosen as shown such that the z axis is pointing out of the plane of the paper. On this collision plane, a positive impact parameter is given by $y=b$. Following this convention, the internuclear axis rotates clockwise as a function of time, and a negative magnetic quantum number corresponds to a clockwise rotation of a classical electron. Thus an electron with $m=-l$, classically, is an electron orbiting clockwise and staying mostly in the collision plane. For each scattering plane, we only consider positive impact parameters.

In experiments where the scattered particles are not measured, the cross sections are obtained by integrating the probabilities over *all* the scattering planes. Let xyz be the natural coordinate system defined above. For collisions occurring on the xy plane, one can calculate the scattering amplitude $A_m(b)$ where m is the magnetic quantum number with respect to the z axis. To obtain total cross sections, it is more convenient to choose the beam axis, which has cylindrical symmetry, as the quantization axis. Let $B_M(b)$ be the scattering amplitude if the quantization axis is along the beam direction, then $B_M(b)$ can be obtained from $A_m(b)$ by a rotation

$$B_M(b)=\sum_m D^l_{mM}(\omega)A_m(b)\ , \tag{1}$$

where ω is a rotation of 90° with respect to the y axis such that the z axis is rotated into the x axis. The cylindrical symmetry with respect to the beam axis allows one to obtain the M-component total cross section

$$\sigma_M=2\pi\int b\,db\,|B_M(b)|^2\ . \tag{2}$$

No such an interpretation is possible for $A_m(b)$ since the z axis depends on the scattering plane. However,

$$\begin{aligned}\sum_M \sigma_M &= \sum_M 2\pi\int b\,db \sum_m D^{l*}_{mM}(\omega)A^*_m(b)\sum_{m'} D^l_{m'M}(\omega)A_{m'}(b)\\ &=\sum_m 2\pi\int b\,db\,|A_m(b)|^2\\ &=\sum_m \rho_m\ ,\end{aligned} \tag{3}$$

where the last equation defines ρ_m. The quantity ρ_m is *not* related directly to any experimental cross section—it is defined as the product of 2π and the integral of the

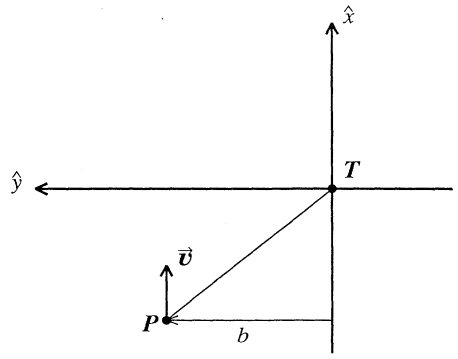

FIG. 1. Natural coordinate system for atomic collisions. The collision plane is the xy plane, with $+x$ being the direction of the incident beam. The quantization axis is the z axis, which is pointing out of the collision plane. For an incident projectile with impact parameter $y=b$, the internuclear axis undergoes a clockwise rotation during the collision.

TABLE I. Electron-capture cross sections and magnetic-substate distributions for $Li^{3+}+H(2s)$ collisions. The cross section to each nl final state is given in units of 10^{-16} cm^2. The substate distributions give the fractional distribution (in %) of each m component within each nl state (see text). The velocities are given in atomic units. Note that m is defined with respect to a quantization axis perpendicular to the scattering plane.

		Distribution					
v	σ_{nl}	$m=-3$	$m=-2$	$m=-1$	$m=0$	$m=1$	$m=2$	$m=3$
				$nl=4f$				
0.8	13.1	97%		2%				
0.6	27.7	89%		7%		2%		
0.4	38.9	82%		13%		3%		1%
0.2	25.9	63%		32%		4%		1%
0.1	10.0	52%		30%		9%		8%
				$nl=4d$				
0.8	4.1		82%		11%		6%	
0.6	15.9		91%		6%		2%	
0.4	32.0		88%		8%		3%	
0.2	17.4		79%		15%		6%	
0.1	11.5		76%		8%		19%	
				$nl=4p$				
0.8	2.9			85%		15%		
0.6	4.1			82%		17%		
0.4	19.5			84%		15%		
0.2	16.8			84%		15%		
0.1	8.2			73%		26%		
				$nl=4s$				
0.8	0.7							
0.6	1.3							
0.4	3.2				100%			
0.2	3.8				100%			
0.1	3.0				100%			

scattering probability over b on any scattering plane. At a given b on the scattering plane, $|A_m(b)|^2$ measures the probability of populating the m substate, and ρ_m is a measure of the total probability over the whole range of b on the scattering plane. If $m=-l$ is the only dominant component, then $\rho_{m=-l}$ gives the total cross section for the *whole* nl state to a good approximation, and from (1), the relative σ_M is determined by the square of the rotation matrix element $|D^l_{M,-l}|^2$. In this paper we will often refer to ρ_m as the magnetic-substate cross section. This should not be confused with the actual experimentally measured quantity, which is σ_M.

III. RESULTS AND DISCUSSION

A. $Li^{3+}+H(2s)$

Electron-capture cross sections for this collision system have been calculated in the velocity range of $v=0.1-0.8$ a.u. The dominant final states populated in this energy range are the $n=4$ states, with $4f$ being the largest. In Fig. 2 we show the $4f$ magnetic-substate populations at $v=0.1$, 0.2, 0.4, and 0.8 (the even reflection symmetry with respect to the collision plane restricts the values of m to $m=-3,-1,+1,+3$ for the $4f$ state). The probabilities for populating the $m=-3$ substate are shown as solid lines, and the $m=-1,1,3$ substate probabilities are shown as dotted, short-dashed, and long-dashed lines, respectively. At $v=0.1$ and 0.2, the $m=-3$ component is the largest, but the $m=-1$ component is also populated significantly. At $v=0.4$ and 0.8, the $m=-3$ component is overwhelmingly the dominant component. Thus the propensity rule states that $m=-l$ is the dominant magnetic substate populated. The rule applies for collisions near the velocity matching region and especially at large impact parameters.

The propensity rule applies to the population of other excited states also. Following the definition of "magnetic-substate cross section" ρ_m as given in Sec. II, we list in Table I the cross section for each final nl state and the percentage of contribution from each ρ_m for $v=0.1-0.8$. For the final $4f$ state, we note that the percentage for $m=-3$ is only 52% at $v=0.1$, but it reaches 89% and 97%, respectively, for $v=0.6$ and 0.8. For the population of the $4d$ state, the $m=-2$ component is about 80% or more for $v=0.4$ to 0.8. The cross sections for the $4p$ state are smaller, but the propensity rule still applies and the $m=-1$ state is the dominant channel.

TABLE II. Electron-capture cross sections and magnetic-substate distributions for $Li^{3+}+H(2p_{\pm1,0})$ collisions. The cross section to each nl final state is given in units of 10^{-16} cm^2. The substate distributions give the fractional distribution (in %) of each m component within each nl state (see text). The velocities are given in atomic units. Note that m is defined with respect to a quantization axis perpendicular to the scattering plane.

Initial state	v	σ_{nl}	Distribution $m=-3$	$m=-2$	$m=-1$	$m=0$	$m=1$
			$nl=4f$				
$2p_{-1}$	0.8	13.5	88%		7%		3%
	0.6	27.3	91%		7%		
	0.4	29.4	88%		8%		
$2p_1$	0.8	5.8	90%		9%		1%
	0.6	12.8	79%		18%		2%
	0.4	17.6	60%		36%		3%
			$nl=4d$				
$2p_{-1}$	0.8	2.5	84%		11%		5%
	0.6	11.1	92%		6%		1%
	0.4	31.7	91%		6%		2%
$2p_1$	0.8	1.9	70%		22%		8%
	0.6	7.3	83%		11%		5%
	0.4	14.8	76%		20%		4%
			$nl=4f$				
$2p_0$	0.8	10.6		89%		10%	
	0.6	32.5		96%		4%	
	0.4	71.4		96%		4%	
$2p_0$	0.8	2.2		90%		10%	
	0.6	4.6		92%		8%	
	0.4	13.6		92%		7%	

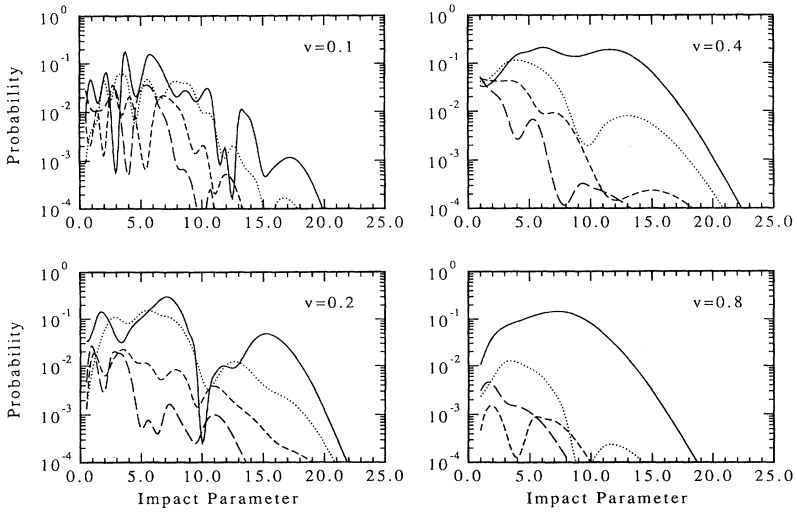

FIG. 2. Electron-capture probabilities $|A_m(b)|^2$ to the $4f$ magnetic substates vs impact parameter b (in a.u.) in Li^{3+} collisions with $H(2s)$ at $v=0.1-0.8$ a.u. Symbols: solid lines, $m=-3$; dotted lines, $m=-1$; short dashed lines, $m=+1$; long dashed lines, $m=+3$. The results show a strong propensity for populating the $m=-3$ state at increasing v.

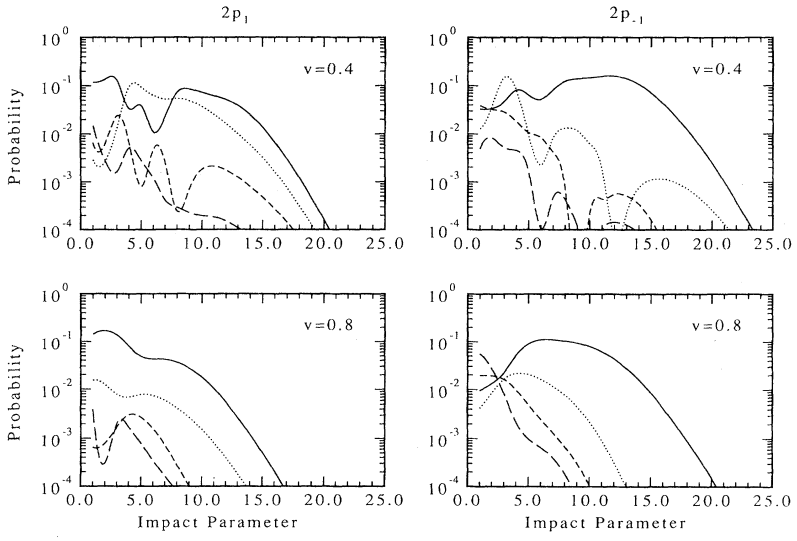

FIG. 3. Same as Fig. 2 but for initial $2p_1$ and $2p_{-1}$ states at $v=0.4$ and 0.8. Note that electron-capture probabilities from the initial $2p_{-1}$ state is larger at a given velocity and occurring at larger impact parameters (in a.u.).

B. $Li^{3+}+H(2p_{\pm1,0})$ collisions

We next examine electron-capture probabilities from oriented initial $2p$ states by Li^{3+}. Following our choice of coordinates, we note that if the electron is initially in the $2p_{-1}$ state, its sense of rotation is the same as the rotation of the internuclear axis. In Fig. 3 we compare the probabilities for electron capture to the $4f$ state for target electrons initially in the $2p_{+1}$ and $2p_{-1}$ states at $v=0.4$ and $v=0.8$. At the same velocity, we note that electron-capture probability and the range of impact parameters with non-negligible probabilities from the $2p_{-1}$ state are much larger than from the $2p_{+1}$ state. For the final states on the projectile, the $m=-l$ substate is predominantly populated by the electron-capture process, irrespective of the orientation of the initial state.

In Table II, we compare the total cross sections for electron capture to $4f$ and $4d$ states and the fractions of contributions from different magnetic components for collisions of protons with hydrogen atoms at two different initial orientations ($2p_{-1}$ and $2p_{+1}$) at $v=0.4$, 0.6, and 0.8. The $m=-l$ component is the dominant substate populated in all cases, and the propensity rule works better for $2p_{-1}$ as the initial state than for $2p_{+1}$ as the initial state at the same collision velocity. We further point out that the propensity rule works better near the velocity matching region.

We next consider collisions where the target is initially in the $2p_0$ state. Because the $2p_0$ wave function is odd under reflection with respect to the scattering plane, the final states populated in the collision must satisfy the condition $l+m=$odd. Therefore the m components that can be populated in the collisions are -2, 0, and $+2$ for $4f$ and -1 and $+1$ for $4d$ states. Our results again show that electron capture populates predominantly the most negative m substate allowed in each nl manifold, as can be seen from Table II, where we compare the total cross

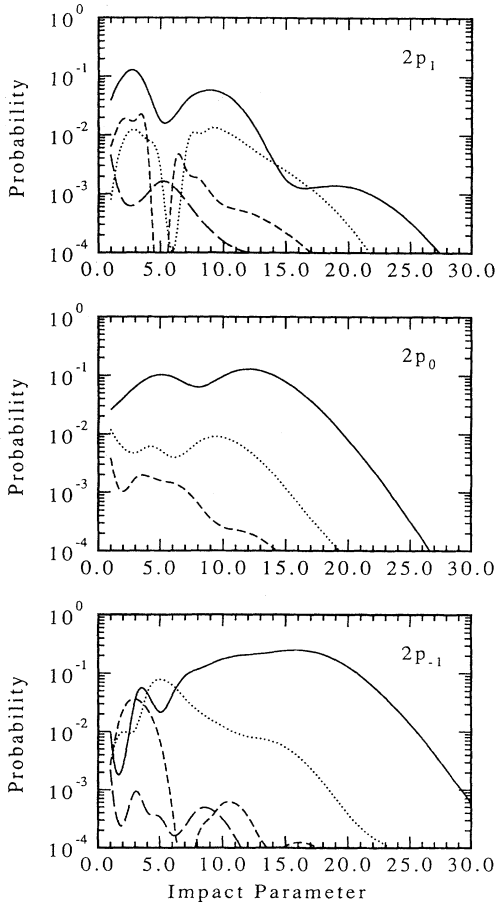

FIG. 4. Electron-capture probabilities to the $4f$ magnetic substates for collisions of He^{2+} with $H(2p_{\pm1,0})$ states at $v=0.4$. Symbols are identical to those in Fig. 2. Note that electron capture from $2p_{-1}$ is the most probable and that it occurs at larger impact parameters (in a.u.).

sections for electron capture to $4f$ and $4d$ states and the contribution from different magnetic components.

C. $He^{2+}+H(2s)$ collisions

For this collision system the electron-capture process populates the $n=3$ and $n=4$ states of He^+ predominantly. In Table III we show the total nl subshell cross sections and the magnetic-substate cross sections for $v=0.1$, 0.2, and 0.4. Clearly the cross section for the $m=-l$ substate is the dominant one within each nl. The velocity dependence also indicates that the propensity rule works better as v approaches the velocity matching ($v=0.5$) region.

TABLE III. Electron-capture cross sections and magnetic-substate distributions for $He^{2+}+H(2s)$ collisions. The cross section to each nl final state is given in units of 10^{-16} cm^2. The substate distributions give the fractional distribution (in %) of each m component within each nl state (see text). The velocities are given in atomic units. Note that m is defined with respect to a quantization axis perpendicular to the scattering plane.

		Distribution					
v	σ_{nl}	$m=-3$	$m=-2$	$m=-1$	$m=0$	$m=1$	$m=2$ $m=3$
				$nl=4f$			
0.4	21.4	95%		2%		2%	1%
0.2	12.8	84%		5%		3%	8%
0.1	7.7	53%		6%		30%	10%
				$nl=4d$			
0.4	19.3		92%		4%		3%
0.2	18.8		78%		13%		8%
0.1	4.8		48%		25%		26%
				$nl=4p$			
0.4	9.6			85%		15%	
0.2	7.6			72%		28%	
0.1	2.9			78%		21%	
				$nl=4s$			
0.4	3.4				100%		
0.2	2.8				100%		
0.1	0.6				100%		
				$nl=3d$			
0.4	34.5		92%		7%		1%
0.2	24.4		71%		23%		6%
0.1	7.3		57%		15%		17%
				$nl=3p$			
0.4	14.8			92%		8%	
0.2	19.1			85%		15%	
0.1	7.7			82%		17%	
				$nl=3s$			
0.4	3.5				100%		
0.2	10.3				100%		
0.1	3.5				100%		

D. Electron capture in $He^{2+}+H(2p_{\pm1})$ collisions

In the velocity range of $v=0.1$–0.4, the dominant final states populated by the electron-capture process for this system are the $n=3$ and 4 states. In Fig. 4 we show the probabilities for electron capture to the different $4f$ magnetic substates at $v=0.4$. The propensity rule dictates that the $m=-3$ magnetic substate should be populated predominantly. From Fig. 4 we note that this rule works very well except for the $2p_1$ initial state where electron-capture probabilities are small and capture occurs only at small impact parameters.

To document the validity of the propensity rule for different final and initial states and the dependence on collision velocities, in Table IV we show the partial electron-capture cross sections from initial $2p_{-1}$ and $2p_1$ states to individual final nl states, and the ρ_m within each l. The comparison is made at two different velocities, $v=0.4$ and 0.2. First, we note that the propensity rule works better for the higher collision velocity. It also

TABLE IV. Electron-capture cross sections and magnetic-substate distributions for $He^{2+}+H(2p_{\pm1})$ collisions. The cross section to each nl final state is given in units of 10^{-16} cm^2. The substate distributions give the fractional distribution (in %) of each m component within each nl state (see text). The velocities are given in atomic units. Note that m is defined with respect to a quantization axis perpendicular to the scattering plane.

			Distribution				
Initial state	v	σ_{nl}	$m=-3$	$m=-2$	$m=-1$	$m=0$	$m=1$ $m=2$ $m=3$
					$nl=4f$		
$2p_{-1}$	0.4	79.9	94%		5%		
	0.2	28.2	88%		6%	3%	3%
$2p_1$	0.4	8.6	77%		17%	4%	
	0.2	9.1	53%		35%	9%	2%
					$nl=4d$		
$2p_{-1}$	0.4	35.6	91%		6%	3%	
	0.2	19.4	67%		18%	15%	
$2p_1$	0.4	5.1	69%		24%	7%	
	0.2	7.6	77%		12%	11%	
					$nl=4p$		
$2p_{-1}$	0.4	10.9	83%		17%		
	0.2	16.4	67%		33%		
$2p_1$	0.4	2.1	72%		28%		
	0.2	2.6	55%		45%		
					$nl=3d$		
$2p_{-1}$	0.4	44.9	95%		5%		
	0.2	27.8	81%		16%	3%	
$2p_1$	0.4	11.5	57%		38%	5%	
	0.2	26.7	81%		13%	6%	
					$nl=3p$		
$2p_{-1}$	0.4	24.7	90%		10%		
	0.2	14.8	75%		25%		
$2p_1$	0.4	6.8	74%		26%		
	0.2	30.9	83%		17%		

works better in general for an initial $2p_{-1}$ state (which has larger cross sections) than for an initial $2p_1$ state. These results are in agreement with the general trends obtained using Li^{3+} projectiles.

IV. SUMMARY AND DISCUSSION

In this article we have examined the propensity rule for populating magnetic substates for electron-capture processes from excited atoms. We have shown that if the quantization axis is chosen to be perpendicular to the scattering plane, the dominant magnetic substate populated for each final nl state is $m=-l$, irrespective of the magnetic quantum number of the initial state. We have examined the propensity rule for electrons initially in the excited $2s$ or oriented $2p$ hydrogenic states and have shown that the propensity rule works exceedingly well despite the degeneracy between the $2s$ and $2p$ states. We have further shown that electron-capture probabilities from initial $2p_{-1}$ states are in general larger than from initial $2p_1$ states. Thus there exists a propensity rule for the dependence of electron-capture probabilities on the orientation of the initial state. We expect that this is true for any ion-atom collision systems. This is in great contrast to the lack of obvious dependence of electron-capture cross sections on the alignment of the initial states.

We conclude by calling attention to the fact that an experimental search for the propensity rule of electron-capture probabilities be carried out for oriented states instead of aligned states. This would require measuring differential electron-capture cross sections at very small scattering angles—a rather difficult task unless the recently developed recoil-ion momentum-spectroscopy technique is applied where the small scattering angles of the projectile are determined by measuring the linear momentum of the recoil ions. We also point out that the dependence of electron-capture probabilities on the initial orientation is expected to be even more pronounced if the angular momentum of the initial excited state is increased, such as in collisions of ions with Rydberg atoms.

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