PHYSICAL REVIEW A VOLUME 16, NUMBER 4 OCTOBER 1977

X-ray and Auger transition probabilities to the 2*p* level of multiply ionized sulfur and chlorine*

Mau Hsiung Chen and Bernd Crasemann
Department of Physics, University of Oregon, Eugene, Oregon 97403

(Received 27 May 1977)

Theoretical multiplet x-ray and Auger rates to the $2p$ level of S and Cl atoms containing one $2p$ hole and a partially filled $3p$ shell have been computed. The initial state is treated in intermediate coupling, and the final state, in LS coupling. Fluorescence yields for each state as well as statistical-average fluorescence yields for each configuration are reported. The spin-orbit interaction is found to have a remarkable effect on the Auger transition probabilities and x-ray fluorescence yields of $2p^53s^23p^n$ configurations; this effect decreases with increasing stages of ionization.

I. INTRODUCTION

Vacancies in a multiply ionized atom couple to form a multiplet structure that strongly influences the decay properties of the system. In particular, we consider an atom that contains an inner-shell hole and a partially filled shell, other shells being filled. The Auger[1] and x-ray[2] transition probabilities to the inner level, and hence, the fluorescence yield[3] of the excited state, can differ by many orders of magnitude among various multiplet states of a given initial hole configuration. This fact has only recently been given theoretical attention.[4-7] Furthermore, a significant effect of the spin-orbit interaction has been predicted for the $2p$ Auger transition probabilities and fluorescence yields of $(2p)^53snl$ configurations of Na and Mg.[8]

Experimental studies of multiplet effects on atomic inner-shell transition probabilities have been scarce and largely limited to Ne and Ar.[9,10] In most experiments, average transition rates are measured in which the different multiplet rates enter with their respective weights; these weights are usually unknown and assumed to be statistical. Only simultaneous high-resolution measurements of x-ray and Auger spectra (and preferably the charge state as well) of multiply ionized atoms (as from beam-foil excitation) can yield detailed evidence on the properties of individual multiplet states. The subject is of fundamental interest as a little-explored aspect of atomic inner-shell physics; it is relevant to applications in connection with the search for states among which a population inversion might be attained with minimal pumping power.

Sulfur and chlorine are likely candidates for experimental investigations of multiplet transition rates.[9] In this paper, we report on calculations of $L_{2,3}$ fluorescence yields and multiplet Auger rates to the $2p$ level of S and Cl atoms containing one $2p$ hole and a partially filled $3p$ shell. The initial state is treated in intermediate coupling, and the final state, in LS coupling. The fluorescence yield for each state J is calculated as

$$\omega(i,J,n)=\frac{\Gamma_R(i,J,n)}{\Gamma_R(i,J,n)+\Gamma_A(i,J,n)}\,. \tag{1}$$

Here, Γ_R and Γ_A are the radiative and Auger widths, respectively; the index n identifies the configuration, and the index i characterizes the initial state. For example, for the $[2p][3p]$ hole-state configuration with $J=1$, there are four states $i=1,2,3,4$.

The average fluorescence yield for a configuration n is

$$\bar{\omega}(n)=\sum_{i,J}C(iJ)\omega(i,J,n)\,, \tag{2}$$

where $C(iJ)$ is the population probability of the state iJ. For a statistical population, we have

$$\bar{\omega}(n)=\frac{\sum_{i,J}(2J+1)\omega(i,J,n)}{\sum_{i,J}(2J+1)}\,. \tag{3}$$

We have computed statistically averaged fluorescence yields both in LS coupling and in intermediate coupling; these are compared in Sec. III.

II. CALCULATIONS

The multiplet transition rates in LS coupling were computed by the same approach taken in our previous work on Ar.[5] The initial hole configuration $[2p][3p]^n$ was coupled via $[2p]\{[3p]^nL_3S_3\}$ LS following Slater.[11] The effect due to the spin-orbit interaction was then included.

The electrostatic matrix elements were taken from Slater's tabulation,[11] and the matrix elements for the spin-orbit interaction were calculated from the expression given by Wybourne[12] for l^Nl' configurations. The relevant F and G Slater integrals and the spin-orbit parameters ξ were calculated using one-electron orbitals corresponding to the appropriate initial configuration, generated by the

TABLE I. Average $L_{2,3}$ Auger and x-ray energies (in eV) for various hole configurations of S and Cl.

Element and configuration	Auger transition energy $L_{2,3}$-M_1M_1	$L_{2,3}$-$M_1M_{2,3}$	$L_{2,3}$-$M_{2,3}M_{2,3}$	X-ray energy
$_{16}$S				
$(2p)^{-1}(3p)^{-2}$	119.0	130.3	141.6	152.6
$(2p)^{-1}(3p)^{-3}$	109.0	120.1	132.6	154.9
$(2p)^{-1}(3p)^{-4}$	98.9	111.1	123.4	158.0
$(2p)^{-1}(3p)^{-5}$	88.9	101.5	...	162.1
$(2p)^{-1}(3p)^{-6}$	79.7	...	...	167.1
$_{17}$Cl				
$(2p)^{-1}(3p)^{-1}$	147.0	160.1	173.1	183.7
$(2p)^{-1}(3p)^{-2}$	135.8	149.3	162.7	187.5
$(2p)^{-1}(3p)^{-3}$	124.5	138.5	152.4	190.7
$(2p)^{-1}(3p)^{-4}$	113.2	127.5	141.9	194.7
$(2p)^{-1}(3p)^{-5}$	102.2	116.8	...	199.5
$(2p)^{-1}(3p)^{-6}$	92.0	...	...	205.4

Herman-Skillman Hartree-Slater approach with $X\alpha$ exchange.[5,13] The resulting $N\times N$ energy matrices including the nondiagonal electrostatic matrix elements were diagonalized to determine eigenvalues and mixing coefficients. The eigenfunction of the ith state with total angular momentum J then is

$$\psi_{i,J}=\sum_{L_3S_3,LS} C_i(L_3S_3,LS,J)\,\psi(L_3S_3,LSJM)\,. \tag{4}$$

For $L_{2,3}$-M_1M_1 Auger transitions, one has the same transition rate for all (i,J) states if the effect due to spectator holes on the transition energies is neglected. For $L_{2,3}$-$M_1M_{2,3}$ and $L_{2,3}$-$M_{2,3}M_{2,3}$ transitions, interference only arises among those components with the same LS quantum numbers but different L_3S_3 quantum numbers. The Auger transition probability from an initial state (i,J) to a final term PQ can be expressed as

$$A(i,J\rightarrow PQ)=\sum_{l_2}\sum_{L''S''}\Big\{\sum_{L'S'}{}' C_i^2(L_3'S_3'L'S'J)\,\big|M(L_3'S_3'L'S'\rightarrow PQl_2\tfrac{1}{2}L''S'')\big|^2 + \sum_{L,S}{}'\Big|\sum_{L_3S_3}C_i(L_3S_3LSJ)\,M(L_3S_3LS\rightarrow PQl_2\tfrac{1}{2}L''S'')\Big|^2\Big\}\,. \tag{5}$$

Here, $|M(L_3S_3LS\rightarrow PQl_2\frac{1}{2}LS)|^2$ is the Auger transition probability in LS coupling[5] and l_2 is the orbital angular momentum of the Auger electron. The summation $L'S'$ is over the terms occuring only once in the wave-function expansion, and the summation LS is over the terms occuring more than once in the same wave-function expansion.

In calculating radiative transition rates $2p^5 3s^2 3p^n\alpha J\rightarrow 2p^6 3s\, 3p^n\alpha' L'S'J'$, one can sum over the possible final states if energy splitting due to the spectator holes is neglected. The total x-ray transition rate then is the same for all (i,J) states; it is given in atomic units by

$$\mathcal{R}_{g1}(i,J)=\tfrac{4}{9}k^3\Big|\int P_{2p}(r)\,r\,P_{3s}(r)\,dr\Big|^2\,, \tag{6}$$

where the wave number k is

$$k=(E_i-E_f)/27.21c\,, \tag{7}$$

with initial and final energies E_i and E_f in eV.

The average x-ray and Auger transition energies were calculated using Slater's transition-state approach[14,15] with the Herman-Skillman Hartree-Slater model[13]; these average energies were used for all multiplet transitions. The Auger and x-ray radial matrix elements were also calculated with

TABLE II. $L_{2,3}$ x-ray transition rates (in multiples of 10^{-7} a.u.) for various hole configurations of S and Cl.

Initial configuration	X-ray transition rate $_{16}$S	$_{17}$Cl
$(2p)^{-1}(3p)^{-1}$	...	6.117
$(2p)^{-1}(3p)^{-2}$	4.362	6.685
$(2p)^{-1}(3p)^{-3}$	4.693	7.195
$(2p)^{-1}(3p)^{-4}$	5.091	7.780
$(2p)^{-1}(3p)^{-5}$	5.580	8.455
$(2p)^{-1}(3p)^{-6}$	6.209	9.317

TABLE III. Relative energy (in eV), Auger transition rates (in multiples of 10^{-3} a.u.), and fluorescence yields (in multiples of 10^{-4}) for sulfur atoms with a $2p$ vacancy in the presence of a partially filled $3p$ shell. The initial state is in intermediate coupling.

Initial hole configuration	Initial state	Relative energy	Auger rate				Fluorescence yield
			$L_{2,3}$-M_1M_1	$L_{2,3}$-$M_1M_{2,3}$	$L_{2,3}$-$M_{2,3}M_{2,3}$	Total	
$(2p)^{-1}(3p)^{-2}$	$J=\frac{1}{2}$						
	1	4.493	0.0521	1.2926	3.6688	5.0135	0.870
	2	2.776	0.0521	0.1458	2.2973	2.4952	1.748
	3	−0.358	0.0521	1.6193	0.0326	1.7041	2.559
	4	−0.694	0.0521	0.0933	0.0294	0.1747	24.903
	5	−1.404	0.0521	0.4897	0.1163	0.6581	6.624
	6	−2.769	0.0521	0.2027	0.0891	0.3438	12.671
	$J=\frac{3}{2}$						
	1	3.922	0.0521	0.7881	5.9640	6.8042	0.641
	2	2.902	0.0521	2.0691	1.7785	3.8997	1.118
	3	2.210	0.0521	2.3728	4.5275	6.9525	0.627
	4	0.697	0.0521	3.0321	5.7353	8.8194	0.495
	5	−0.151	0.0521	1.4309	0.7989	2.2818	1.911
	6	−0.905	0.0521	0.5753	0.4937	1.1211	3.889
	7	−1.447	0.0521	0.2703	0.1734	0.4958	8.790
	8	−1.727	0.0521	0.1325	0.1573	0.3419	12.743
	$J=\frac{5}{2}$						
	1	2.566	0.0521	3.2027	6.0211	9.2759	0.470
	2	0.953	0.0521	0.1730	0.4326	0.6577	6.628
	3	−0.820	0.0521	0.1061	0.1451	0.3033	14.362
	4	−1.768	0.0521	0.0837	0.0657	0.2015	21.602
	5	−2.041	0.0521	0.0704	0.1058	0.2283	19.068
	$J=\frac{7}{2}$						
	1	−0.106	0.0521	0.0028	0.1352	0.1901	22.895
	2	−2.324	0.0521	0.0606	0.1108	0.2235	19.477
$(2p)^{-1}(3p)^{-3}$	$J=0$						
	1	7.146	0.0586	5.1982	5.8864	11.1433	0.421
	2	3.498	0.0586	0.2079	6.7045	6.9711	0.673
	3	1.663	0.0586	4.9370	0.8863	5.8820	0.798
	4	−2.951	0.0586	0.4709	0.0056	0.5351	8.763
	$J=1$						
	1	3.653	0.0586	0.1923	6.3715	6.6224	0.709
	2	2.204	0.0586	0.1857	0.1490	0.3934	11.917
	3	1.967	0.0586	4.2364	0.8280	5.1230	0.916
	4	1.520	0.0586	0.3297	0.1757	0.5639	8.315
	5	0.570	0.0586	0.2862	0.0225	0.3672	12.763
	6	−0.749	0.0586	0.2577	0.0955	0.4118	11.384
	7	−1.661	0.0586	0.0741	0.0679	0.2007	23.332
	8	−2.447	0.0586	0.2569	0.0057	0.3212	14.589
	9	−3.303	0.0586	0.2552	0.0124	0.3261	14.369
	$J=2$						
	1	4.973	0.0586	5.1505	6.5374	11.7465	0.400
	2	3.632	0.0586	0.8962	6.8277	7.7824	0.603
	3	2.096	0.0586	1.5341	0.6193	2.2120	2.121
	4	1.801	0.0586	2.4551	0.1808	2.6945	1.741
	5	1.120	0.0586	0.1071	0.0972	0.2629	17.816
	6	−0.025	0.0586	0.0817	0.1358	0.2762	16.965
	7	−1.128	0.0586	0.2603	0.0977	0.4165	11.254
	8	−2.152	0.0586	0.3565	0.0171	0.4322	10.847
	9	−3.667	0.0586	0.1621	0.0177	0.2384	19.651

TABLE III. (*Continued*)

Initial hole configuration	Initial state	Relative energy	Auger rate			Total	Fluorescence yield
			$L_{2,3}$-M_1M_1	$L_{2,3}$-$M_1M_{2,3}$	$L_{2,3}$-$M_{2,3}M_{2,3}$		
	$J=3$						
	1	0.799	0.0586	0.0043	0.0458	0.1088	42.961
	2	0.254	0.0586	0.0193	0.1076	0.1855	25.233
	3	−0.939	0.0586	0.0044	0.1080	0.1711	27.360
	4	−1.438	0.0586	0.1004	0.0602	0.2192	21.362
	5	−4.090	0.0586	0.0610	0.0000	0.1197	39.059
	$J=4$						
	$^3F_4$	−1.108	0.0586	0.0021	0.1082	0.1689	27.709
$(2p)^{-1}(3p)^{-4}$	$J=\frac{1}{2}$						
	1	5.956	0.0659	0.2817	4.9279	5.2755	0.965
	2	4.244	0.0659	0.3773	0.3094	0.7526	6.760
	3	0.048	0.0659	0.0274	0.0053	0.0987	51.333
	4	−0.818	0.0659	0.6371	0.0205	0.7235	7.032
	5	−1.722	0.0659	5.8444	0.0087	5.9190	0.860
	6	−2.354	0.0659	0.7346	0.0001	0.8006	6.355
	$J=\frac{3}{2}$						
	1	6.229	0.0659	0.3693	5.1972	5.6324	0.904
	2	3.266	0.0659	0.0490	0.0149	0.1298	39.077
	3	1.680	0.0659	0.2899	0.0220	0.3779	13.455
	4	0.075	0.0659	0.2951	0.0217	0.3827	13.286
	5	−0.459	0.0659	0.3832	0.0074	0.4565	11.140
	6	−1.440	0.0659	3.6282	0.0065	3.7006	1.376
	7	−1.532	0.0659	2.3994	0.0012	2.4665	2.064
	8	−2.583	0.0659	0.4913	0.0009	0.5582	9.113
	$J=\frac{5}{2}$						
	1	1.683	0.0659	0.0008	0.0308	0.0975	51.934
	2	0.474	0.0659	0.0013	0.0632	0.1305	38.868
	3	−0.144	0.0659	0.0067	0.0002	0.0728	69.465
	4	−1.696	0.0659	0.0053	0.0000	0.0712	70.949
	5	−2.784	0.0659	0.1312	0.0000	0.1971	25.767
	$J=\frac{7}{2}$						
	1	−0.186	0.0659	0.0016	0.0941	0.1616	31.398
	2	−1.921	0.0659	0.0007	0.0002	0.0667	75.711
$(2p)^{-1}(3p)^{-5}$	$J=0$						
	1	8.258	0.0741	9.9597		10.0338	0.556
	2	0.800	0.0741	0.0580		0.1321	42.068
	$J=1$						
	1	1.061	0.0741	0.0103		0.0844	65.695
	2	0.330	0.0741	0.0002		0.0743	74.557
	3	−1.332	0.0741	0.0008		0.0749	73.909
	4	−2.243	0.0741	0.2277		0.3018	18.453
	$J=2$						
	1	0.972	0.0741	0.0007		0.0748	74.068
	2	−0.017	0.0741	0.0005		0.0746	74.270
	3	−0.813	0.0741	0.0006		0.0747	74.172
	$J=3$						
	$^3D_3$	−0.973	0.0741	0.0004		0.0745	74.304
$(2p)^{-1}(3p)^{-6}$	^2P		0.0850			0.0850	72.510

TABLE IV. Relative energy (in eV), Auger transition rates (in multiples of 10^{-3} a.u.), and fluorescence yields (in multiples of 10^{-4}) for chlorine atoms with a $2p$ vacancy in the presence of a partially filled $3p$ shell. The initial state is in intermediate coupling.

Initial hole configuration	Initial state	Relative energy	Auger rate			Total	Fluorescence yield
			$L_{2,3}$-M_1M_1	$L_{2,3}$-$M_1M_{2,3}$	$L_{2,3}$-$M_{2,3}M_{2,3}$		
$(2p)^{-1}(3p)^{-1}$	$J=0$						
	1	4.166	0.0579	2.3512	5.2429	7.6520	0.799
	2	1.096	0.0579	2.4388	6.2223	8.7190	0.702
	$J=1$						
	1	1.471	0.0579	1.9903	5.1369	7.1851	0.851
	2	0.253	0.0579	0.0663	0.1795	0.3037	20.101
	3	−0.507	0.0579	0.4812	1.1535	1.6926	3.613
	4	−1.940	0.0579	0.0806	0.2223	0.3607	16.929
	$J=2$						
	1	2.318	0.0579	2.2063	5.6031	7.8673	0.777
	2	0.353	0.0579	2.3436	6.0576	8.4591	0.723
	3	−0.944	0.0579	0.2964	0.7893	1.1436	5.346
	$J=3$						
	$^3D_3$	−1.675	0.0579	0.0564	0.1744	0.2887	21.142
$(2p)^{-1}(3p)^{-2}$	$J=\frac{1}{2}$						
	1	5.486	0.0644	1.5416	4.9052	6.5112	1.027
	2	3.439	0.0644	0.1749	2.8053	3.0445	2.195
	3	−0.441	0.0644	1.7992	0.0409	1.9045	3.509
	4	−0.789	0.0644	0.2742	0.0382	0.3768	17.709
	5	−1.876	0.0644	0.5548	0.1483	0.7675	8.702
	6	−3.427	0.0644	0.2495	0.1199	0.4338	15.387
	$J=\frac{3}{2}$						
	1	4.897	0.0644	0.9387	7.6719	8.6750	0.771
	2	3.475	0.0644	2.7377	2.9877	5.7899	1.154
	3	2.691	0.0644	2.6571	5.2178	7.9394	0.842
	4	0.931	0.0644	3.5707	7.4250	11.0600	0.604
	5	−0.132	0.0644	1.5257	0.9444	2.5346	2.637
	6	−1.077	0.0644	0.7993	0.7530	1.6167	4.133
	7	−1.798	0.0644	0.3399	0.2093	0.6135	10.884
	8	−2.109	0.0644	0.1664	0.2003	0.4312	15.480
	$J=\frac{5}{2}$						
	1	3.219	0.0644	3.8041	7.7595	11.6280	0.575
	2	1.210	0.0644	0.2069	0.5506	0.8219	8.127
	3	−0.979	0.0644	0.1438	0.2233	0.4315	15.470
	4	−2.232	0.0644	0.995	0.0796	0.2435	27.380
	5	−2.519	0.0644	0.0856	0.1304	0.2804	23.782
	$J=\frac{7}{2}$						
	1	−0.225	0.0644	0.0018	0.1660	0.2321	28.717
	2	−2.901	0.0644	0.0742	0.1378	0.2764	24.129
$(2p)^{-1}(2p)^{-3}$	$J=0$						
	1	8.650	0.0718	5.9950	7.2334	13.3003	0.541
	2	4.298	0.0718	0.2780	8.4928	8.8426	0.814
	3	1.968	0.0718	5.7206	0.9480	6.7404	1.067
	4	−3.411	0.0718	0.4931	0.0021	0.5670	12.675
	$J=1$						
	1	4.530	0.0718	0.2641	7.9750	8.3110	0.866
	2	2.674	0.0718	0.2353	0.1795	0.4866	14.765
	3	2.395	0.0718	4.8320	0.8974	5.8012	1.240
	4	1.776	0.0718	0.3851	0.2661	0.7230	9.942
	5	0.556	0.0718	0.3481	0.0329	0.4529	15.863
	6	−0.901	0.0718	0.3417	0.1151	0.5286	13.594
	7	−2.067	0.0718	0.0927	0.0864	0.2509	28.591
	8	−2.670	0.0718	0.2104	0.0306	0.3128	22.950
	9	−3.756	0.0718	0.3198	0.0071	0.3987	18.013
	$J=2$						
	1	6.080	0.0718	5.9487	8.0315	14.0520	0.512
	2	4.537	0.0718	1.2055	8.4081	9.6854	0.743

TABLE IV. (*Continued*)

Initial hole configuration	Initial state	Relative energy		Auger rate			Fluorescence yield
			$L_{2,3}$-M_1M_1	$L_{2,3}$-$M_1M_{2,3}$	$L_{2,3}$-$M_{2,3}M_{2,3}$	Total	
	3	2.543	0.0718	1.8599	0.6876	2.6194	2.746
	4	2.097	0.0718	2.5810	0.3492	3.0020	2.396
	5	1.262	0.0718	0.1178	0.1425	0.3321	21.620
	6	0.025	0.0718	0.1198	0.1638	0.3553	20.208
	7	−1.361	0.0718	0.3611	0.1153	0.5481	13.110
	8	−2.364	0.0718	0.3172	0.0660	0.4550	15.788
	9	−4.181	0.0718	0.2006	0.0190	0.2914	24.633
	$J=3$						
	1	0.883	0.0718	0.0019	0.0567	0.1304	54.875
	2	0.353	0.0718	0.0242	0.1246	0.2205	32.523
	3	−1.202	0.0718	0.0034	0.1269	0.2021	35.472
	4	−1.807	0.0718	0.1215	0.0732	0.2664	26.932
	5	−4.718	0.0718	0.0740	0.0001	0.1459	49.083
	$J=4$						
	$^3F_4$	−1.406	0.0718	0.0013	0.1269	0.2000	35.841
$(2p)^{-1}(3p)^{-4}$	$J=\frac{1}{2}$						
	1	7.086	0.0796	0.3434	5.9059	6.3289	1.229
	2	5.036	0.0796	0.4506	0.3272	0.8574	9.065
	3	0.141	0.0796	0.0305	0.0078	0.1178	65.590
	4	−0.863	0.0796	0.6401	0.0315	0.7512	10.346
	5	−2.079	0.0796	6.3441	0.0152	6.4389	1.208
	6	−2.812	0.0796	1.1603	0.0000	1.2399	6.271
	$J=\frac{3}{2}$						
	1	7.508	0.0796	0.4447	6.1669	6.6911	1.163
	2	3.699	0.0796	0.0315	0.0357	0.1468	52.716
	3	2.009	0.0796	0.4188	0.0243	0.5226	14.864
	4	0.185	0.0796	0.3395	0.0341	0.4531	17.141
	5	−0.418	0.0796	0.4364	0.0127	0.5287	14.695
	6	−1.757	0.0796	3.4027	0.0095	3.4918	2.228
	7	−1.852	0.0796	3.2256	0.0037	3.3089	2.351
	8	−3.112	0.0796	0.6708	0.0008	0.7512	10.346
	$J=\frac{5}{2}$						
	1	2.068	0.0796	0.0007	0.0397	0.1201	64.386
	2	0.498	0.0796	0.0012	0.0661	0.1470	52.662
	3	−0.013	0.0796	0.0066	0.0009	0.0871	88.581
	4	−2.035	0.0796	0.0067	0.0000	0.0863	89.307
	5	−3.344	0.0796	0.1536	0.0000	0.2332	33.257
	$J=\frac{7}{2}$						
	1	−0.332	0.0796	0.0010	0.1064	0.1871	41.420
	2	−2.308	0.0796	0.0008	0.0003	0.0807	95.476
$(2p)^{-1}(3p)^{-5}$	$J=0$						
	1	9.770	0.0879	11.0709		11.1588	0.758
	2	0.986	0.0879	0.0809		0.1688	49.829
	$J=1$						
	1	1.378	0.0879	0.0144		0.1023	81.988
	2	0.779	0.0879	0.0003		0.0882	94.984
	3	−0.520	0.0879	0.0010		0.0889	94.195
	4	−2.696	0.0879	0.2623		0.3502	24.084
	$J=2$						
	1	1.295	0.0879	0.0002		0.0881	95.046
	2	−0.072	0.0879	0.0001		0.0880	95.218
	3	−1.051	0.0879	0.0004		0.0883	94.804
	$J=3$						
	$^3D_3$	−1.206	0.0879	0.0006		0.0885	94.669
$(2p)^{-1}(3p)^{-6}$	^2P		0.0987			0.0987	93.674

TABLE V. Statistically averaged $L_{2,3}$ fluorescence yields (in multiples of 10^{-4}) for various hole configurations of S, Cl, and Ar. Theoretical results are given both for *LS* coupling and for intermediate coupling of the initial state.

Initial hole	Sulfur		Chlorine		Argon		
configuration	*LS*	Intermediate	*LS*	Intermediate	*LS*[a]	Intermediate[b]	Experiment[c]
$(2p)^{-1}(3p)^{-1}$	⋯	⋯	14.918	8.561	17.97	10.31	5.4 ±1.3
$(2p)^{-1}(3p)^{-2}$	14.378	10.348	17.901	12.421	24.83	17.23	25 ±10
$(2p)^{-1}(3p)^{-3}$	20.092	17.114	25.672	21.801	37.84	32.13	30 ±9
$(2p)^{-1}(3p)^{-4}$	47.218	32.300	60.353	41.264	79.61	54.43	
$(2p)^{-1}(3p)^{-5}$	67.591	65.921	86.351	84.010	112.16	109.20	
$(2p)^{-1}(3p)^{-6}$	72.510		93.635				

[a] From Ref. 5.

[b] Obtained by multiplying the *LS*-coupling values by the reduction factors for $_{17}$Cl.

[c] From Ref. 16.

Herman-Skillman wave functions,[13] using $X\alpha$ exchange.[5]

III. RESULTS AND DISCUSSION

The calculated average Auger and x-ray energies for the decay of S and Cl $(2p)^{-1}(3p)^{-n}$ configurations are listed in Table I. The theoretical $L_{2,3}$ x-ray transition rates are listed in Table II. Relative initial-state energies, Auger transition rates, and fluorescence yields are listed in Table III for $_{16}$S and in Table IV for $_{17}$Cl; these quantities were computed with the initial state expressed in intermediate coupling. The various initial states are listed in Tables III and IV in order of decreasing energies.

The statistically averaged fluorescence yields for each configuration $2p^5 3s^2 3p^n$ are listed in Table V, as calculated both in *LS* and in intermediate coupling. The effect of the spin-orbit interaction on the Auger transition probabilities and x-ray fluorescence yields of $2p^5 3s^2 3p^n$ configurations is seen to be remarkable, consistent with the findings of McGuire[8] on Na and Mg. This effect decreases with higher stages of ionization.

The reduction factors for the average fluorescence yields from *LS* coupling to intermediate coupling change so slowly in going from S to Cl that they can be applied to our earlier results for Ar,[5] for which experimental values are available for comparison.[16] These fluorescence yields have been included in Table V.

---

*Work supported in part by the U. S. Army Research Office (Grant No. DAHC04-75-G-0021) and by the National Aeronautics and Space Administration (Grant No. NGR 38-003-036).

[1] E. J. McGuire, in *Atomic Inner-Shell Processes*, edited by B. Crasemann (Academic, New York, 1975), Vol. 1, p. 293.

[2] J. H. Scofield, in Ref. 1, Vol. 1, p. 265.

[3] W. Bambynek, B. Crasemann, R. W. Fink, H.-U. Freund, Hans Mark, C. D. Swift, R. E. Price, and P. Venugopala Rao, Rev. Mod. Phys. 44, 716 (1972).

[4] E. J. McGuire, Phys. Rev. A 10, 32 (1974).

[5] M. H. Chen and B. Crasemann, Phys. Rev. A 10, 2232 (1974).

[6] M. H. Chen and B. Crasemann, Phys. Rev. A 12, 959 (1975).

[7] C. P. Bhalla, Phys. Rev. A 12, 122 (1975).

[8] E. J. McGuire, Phys. Rev. A 14, 1402 (1976).

[9] R. J. Fortner, Phys. Rev. A 10, 2218 (1974).

[10] K.-O. Groeneveld, R. Mann, G. Nolts, S. Schumann, R. Spohr, and B. Fricke, Z. Phys. A 274, 191 (1975).

[11] J. C. Slater, *Quantum Theory of Atomic Structure* (McGraw-Hill, New York, 1960).

[12] B. G. Wybourne, *Spectroscopic Properties of Rare Earths* (Wiley, New York, 1965), Eq. (2-110).

[13] F. Herman and S. Skillman, *Atomic Structure Calculations* (Prentice-Hall, Englewood Cliffs, N. J., 1963).

[14] L. I Yin, I. Adler, T. Tsang, M. H. Chen, D. A. Ringers, and B. Crasemann, Phys. Rev. A 9, 1070 (1974).

[15] J. C. Slater, *Quantum Theory of Molecules and Solids, Vol. 4: The Self-Consistent Field for Molecules and Solids* (McGraw-Hill, New York, 1974).

[16] A. Langenberg, F. J. de Heer, and J. van Eck, *Electronic and Atomic Collisions, Abstracts of Papers of the Ninth International Conference on the Physics of Electronic and Atomic Collisions*, edited by J. S. Risley and R. Geballe (University of Washington, Seattle, 1975), Vol. 2, p. 935.