

HARTREE-SLATER SUBSHELL PHOTOIONIZATION CROSS-SECTIONS AT 1254 AND 1487 eV

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(First received 27 June 1975; in final form 20 August 1975)

ABSTRACT

The results of calculations of photoelectric cross-sections for the $K\alpha$ lines of magnesium at 1254 eV and of aluminum at 1487 eV are presented. All of the subshell cross-sections are given for Z values up to 96. The calculations were carried out relativistically using the single-potential Hartree–Slater atomic model.

This paper presents calculated subshell photoionization cross-sections for all Z values up to 96 for the energies of the $K\alpha$ emission lines of magnesium at 1254 eV and of aluminum at 1487 eV. The cross-sections were calculated using transition matrix elements with the electrons in the initial and final states treated as moving in the same Hartree–Slater potential. The potential was determined self consistently for the neutral-atom occupations of the subshells with the potential introduced by Slater¹ used to approximate the effect of exchange. The relativistic formulation of the calculation was used with the calculated binding energies used for the ionization energies and the coefficient of the exchange potential given by Slater¹. With the necessary modifications to treat the continuum states, the treatment follows that used previously for the calculation of the characteristic X-ray emission rates².

The total and subshell cross-sections are presented in Tables 1 and 2 relative to the calculated values for the ionization of the 1s state of carbon of 22,200 barns at 1254 eV and 13,600 barns at 1487 eV. The 1487 eV data have previously been presented in graphical form by Carter et al.³ and that at 1254 eV by Swingle⁴. The model uses single particle states in a central potential to represent the atomic states. Within the model the only accessible final states are those with a single vacancy out of the initial configuration. In general the single particle states will be split into a number of components and multiple excitations can also occur. If the multiplet splittings are not too great, the calculated cross-sections should give the sum over all the multiplets from a given vacancy state and all excitations in the outer orbitals. If j–j coupling is not valid, i.e. the splittings are large enough to mix the different

Table 1. Photoionization cross sections at 1254 eV in units of the C 1s cross section of 22,200 barns.

Z	Total	1s1/2	2s1/2	2p1/2	2p3/2	3s1/2	3p1/2	3p3/2	3d3/2	3d5/2	4s1/2	4p1/2	4p3/2
H	1	0.0002	0.0002										
He	2	0.0087	0.0087										
Li	3	0.0602	0.0593										
Be	4	0.207	0.1997	0.0008									
B	5	0.515	0.492	0.0074									
C	6	1.05	1.00	0.0470	0.0001	0.0002							
N	7	1.87	1.77	0.0841	0.0006	0.0012							
O	8	3.01	2.85	0.1345	0.0025	0.0049							
F	9	4.51	4.26	0.1968	0.0073	0.0145							
Ne	10	6.34	5.95	0.277	0.0381	0.0751							
Na	11	8.60	7.99	0.390	0.0714	0.1406	0.0059						
Mg	12	0.912	0.525	0.1214	0.239	0.0261							
Al	13	1.31	0.681	0.1935	0.380	0.0485							
Si	14	1.81	0.855	0.292	0.573	0.0726	0.0012	0.0023					
P	15	2.43	1.05	0.422	0.828	0.0998	0.0050	0.0097					
S	16	3.21	1.25	0.590	1.15	0.1302	0.0129	0.0253					
Cl	17	4.15	1.48	0.800	1.56	0.1632	0.0269	0.0527					
Ar	18	5.28	1.71	1.06	2.07	0.1989	0.0493	0.0964					
K	19	6.61	1.95	1.37	2.67	0.249	0.0823	0.1605					
Ca	20	8.17	2.21	1.74	3.39	0.305	0.1221	0.238			0.0061		
							0.1693	0.330			0.0233		
Sc	21	9.90	2.46	2.18	4.24	0.356	0.216	0.420	0.0020	0.0030			
Ti	22	11.87	2.72	2.68	5.22	0.408	0.268	0.521	0.0064	0.0095	0.0273		
V	23	14.06	2.98	3.26	6.33	0.462	0.326	0.633	0.0195	0.0213	0.0308		
Cr	24	16.47	3.23	3.92	7.60	0.511	0.382	0.740	0.0303	0.0445	0.0339		
Mn	25	19.18	3.48	4.63	8.99	0.575	0.460	0.892	0.0484	0.0711	0.0398		
Fe	26	22.11	3.70	5.43	10.54	0.634	0.535	1.04	0.0788	0.1156	0.0425		
Co	27	25.25	3.92	6.28	12.20	0.693	0.616	1.19	0.1220	0.1787	0.0451		
Ni	28	28.56	4.16	7.18	13.92	0.753	0.701	1.36	0.1814	0.265	0.0476		
Cu	29	32.18	4.38	8.18	15.87	0.805	0.779	1.50	0.268	0.390	0.0788		
Zn	30	36.25	4.55	9.29	18.01	0.873	0.882	1.70	0.365	0.532	0.0520		
Ga	31	36.17		10.56	20.47	0.945	0.993	1.92	0.485	0.708	0.0742	0.0056	0.0106
Ge	32	27.20			21.22	1.02	1.11	2.15	0.631	0.920	0.0939	0.0179	0.0340
As	33	6.92				1.10	1.24	2.40	0.802	1.17	0.1137	0.0372	0.0710
Se	34	7.99				1.18	1.37	2.65	1.00	1.46	0.1343	0.0642	0.1228
Br	35	9.17				1.26	1.50	2.92	1.24	1.80	0.1557	0.0996	0.1906
Kr	36	10.48				1.35	1.64	3.20	1.50	2.19	0.1779	0.1441	0.276
Rb	37	11.91				1.43	1.79	3.48	1.81	2.63	0.209	0.1868	0.361
Sr	38	13.47				1.52	1.93	3.78	2.15	3.14	0.242	0.230	0.445
Y	39	15.14				1.61	2.08	4.09	2.54	3.70	0.273	0.268	0.521
Zr	40	16.96				1.70	2.24	4.40	2.97	4.33	0.305	0.307	0.596
Nb	41	18.90				1.79	2.39	4.71	3.45	5.01	0.333	0.340	0.661
Mo	42	21.01				1.89	2.54	5.03	3.97	5.77	0.364	0.379	0.739
Tc	43	23.28				1.98	2.69	5.36	4.54	6.60	0.397	0.419	0.818
Ru	44	25.71				2.07	2.84	5.68	5.17	7.51	0.429	0.460	0.899
Rh	45	28.32				2.15	2.98	6.00	5.84	8.48	0.463	0.501	0.981
Pd	46	31.10				2.24	3.12	6.33	6.58	9.54	0.494	0.538	1.06
Ag	47	34.06				2.33	3.25	6.64	7.36	10.68	0.531	0.586	1.15
Cd	48	37.20				2.40	3.39	6.96	8.22	11.91	0.571	0.636	1.26

Table 1 (continued). Cross sections at 1254 eV in units of 22,200 barns.

Z	Total	3s1/2	3p1/2	3p3/2	3d3/2	3d5/2	4s1/2	4p1/2	4p3/2	4d3/2	4d5/2	4f5/2	4f7/2
In	49	40.54	2.48	3.51	7.27	9.13	13.23	0.611	0.689	1.37	0.893	1.29	
Sn	50	44.02	2.54	3.62	7.58	10.09	14.63	0.653	0.743	1.48	1.05	1.51	
Sb	51	47.69	2.60	3.71	7.86	11.13	16.13	0.696	0.799	1.60	1.22	1.76	
Te	52	51.51	2.67	3.79	8.14	12.21	17.70	0.741	0.856	1.73	1.40	2.01	
I	53	55.43	2.75	3.87	8.37	13.33	19.33	0.785	0.913	1.86	1.58	2.29	
Xe	54	59.64	2.83	3.95	8.64	14.55	21.08	0.831	0.971	1.99	1.78	2.57	
Cs	55	64.02	2.84	4.04	8.94	15.80	22.93	0.877	1.03	2.12	1.99	2.88	
Ba	56	65.53		4.10	9.26	17.04	24.75	0.924	1.09	2.26	2.21	3.20	
La	57	69.64		4.06	9.52	18.25	26.49	0.971	1.15	2.40	2.44	3.53	
Ce	58	69.82			9.67	19.67	28.57	1.00	1.18	2.49	2.58	3.74	0.0689
Pr	59	74.30			9.75	21.13	30.72	1.04	1.23	2.60	2.77	4.01	0.1256
Nd	60	69.16				22.56	32.96	1.07	1.27	2.71	2.96	4.28	0.200
Pm	61	74.06											
Sm	62	79.35				24.32	35.33	1.11	1.30	2.81	3.14	4.55	0.296
Eu	63	85.36				26.12	37.90	1.14	1.34	2.91	3.33	4.82	0.416
Gd	64	85.24				28.20	40.87	1.17	1.37	3.01	3.51	5.09	0.562
Tb	65	39.20				43.43		1.20	1.41	3.13	3.73	5.41	0.693
Dy	66	19.55				20.80		1.22	1.43	3.21	3.88	5.61	0.949
Ho	67	20.78						1.25	1.45	3.30	4.05	5.87	1.20
Er	68	22.09						1.27	1.47	3.39	4.22	6.13	1.49
Tm	69	23.48						1.29	1.49	3.48	4.39	6.37	1.82
Yb	70	24.97						1.31	1.50	3.56	4.56	6.62	2.20
								1.32	1.51	3.64	4.72	6.85	2.63
Lu	71	26.65						1.34	1.52	3.73	4.91	7.13	3.05
Hf	72	28.45						1.36	1.53	3.83	5.10	7.42	3.50
Ta	73	30.35						1.38	1.54	3.93	5.29	7.71	3.99
W	74	32.36						1.39	1.55	4.03	5.48	8.01	4.52
Re	75	34.48						1.41	1.55	4.13	5.67	8.31	5.08
Os	76	36.70						1.42	1.55	4.24	5.86	8.60	5.67
Ir	77	39.08						1.43	1.55	4.34	6.05	8.90	6.30
Pt	78	41.50						1.44	1.55	4.45	6.24	9.20	6.97
Au	79	44.03						1.45	1.53	4.55	6.42	9.50	7.68
Hg	80	46.63						1.45	1.52	4.65	6.60	9.79	8.43
Tl	81	49.35						1.46	1.50	4.75	6.78	10.08	9.22
Pb	82	52.15						1.46	1.47	4.86	6.94	10.37	10.05
Bi	83	55.03						1.45	1.45	4.96	7.11	10.64	10.93
Po	84	58.01						1.44	1.42	5.06	7.27	10.92	11.84
At	85	61.08						1.44	1.38	5.15	7.42	11.20	12.80
Rn	86	64.22						1.44	1.34	5.24	7.56	11.46	13.80
Fr	87	67.45						1.44	1.30	5.34	7.69	11.70	14.84
Ra	88	70.74						1.44	1.26	5.42	7.82	11.95	15.92
Ac	89	74.34						1.41	1.22	5.50	7.95	12.21	17.05
Th	90	76.27						1.58	1.17	5.59	8.05	12.45	18.21
Pa	91	79.91						1.12	5.68	8.13	12.66	19.38	24.81
U	92	82.57							5.77	8.21	12.84	20.61	26.38
Np	93	86.49							5.87	8.31	13.02	21.87	28.02
Pu	94	90.56							5.95	8.39	13.22	23.14	29.67
Am	95	94.61							6.03	8.43	13.43	24.44	31.35
Cm	96	98.65							6.08	8.45	13.57	25.80	33.09

Table 1 (continued). Cross sections at 1254 eV in units of 22,200 barns.

Z	5s1/2	5p1/2	5p3/2	5d3/2	5d5/2	5f5/2	5f7/2	6s1/2	6p1/2	6p3/2	6d3/2	6d5/2	7s1/2
In	49	0.0626	0.0058	0.0107									
Sn	50	0.0765	0.0169	0.0318									
Sb	51	0.0899	0.0331	0.0629									
Te	52	0.1036	0.0542	0.1040									
I	53	0.1175	0.0805	0.1555									
Xe	54	0.1319	0.1123	0.218				0.0049					
Cs	55	0.1523	0.1397	0.278				0.0171					
Ba	56	0.1737	0.1661	0.334				0.0206					
La	57	0.1933	0.1887	0.362				0.0178					
Ce	58	0.1891	0.1805	0.365				0.0181					
Pr	59	0.1958	0.1864	0.378				0.0183					
Nd	60	0.202	0.1917	0.390									
Pm	61	0.208	0.1964										
Sm	62	0.213	0.201	0.402				0.0184					
Eu	63	0.219	0.205	0.422				0.0186					
Gd	64	0.235	0.223	0.465				0.0187					
Tb	65	0.228	0.211	0.440				0.0222					
Dy	66	0.232	0.214	0.449				0.0189					
Ho	67	0.237	0.216	0.457				0.0189					
Er	68	0.240	0.219	0.464				0.0190					
Tm	69	0.244	0.220	0.471				0.0190					
Yb	70	0.247	0.222	0.478				0.0191					
Lu	71	0.261	0.237	0.519									
Hf	72	0.276	0.253	0.562	0.0290			0.0231					
Ta	73	0.291	0.268	0.606	0.0747			0.0261					
W	74	0.306	0.283	0.651	0.1357			0.0287					
Re	75	0.322	0.299	0.697	0.212			0.0310					
Os	76	0.337	0.314	0.743	0.303			0.0330					
Ir	77	0.350	0.324	0.774	0.410			0.0349					
Pt	78	0.366	0.340	0.829	0.593								
Au	79	0.381	0.353	0.877	0.709			0.0167					
Hg	80	0.397	0.368	0.935	0.855			0.0173					
Tl	81	0.413	0.383	0.996	0.707			0.0410					
Pb	82	0.430	0.398	1.06	0.804								
Bi	83	0.446	0.412	1.13	0.900			0.0513	0.0042	0.0079			
Po	84	0.462	0.426	1.19	0.997			0.0597	0.0115	0.0233			
At	85	0.478	0.439	1.26	1.09			0.0676	0.0210	0.0456			
Rn	86	0.493	0.451	1.33	1.19			0.0753	0.0329	0.0745			
Fr	87	0.508	0.462	1.40	1.29			0.0830	0.0469	0.1099			
Ra	88	0.523	0.472	1.48	1.39			0.0906	0.0631	0.1520			0.0037
Ac	89	0.537	0.480	1.55	1.49			0.1008	0.0738	0.1928			0.0122
Th	90	0.551	0.488	1.63	1.60			0.1109	0.0837	0.230			0.0152
					2.36			0.1207	0.0925	0.262	0.0125	0.0174	
					2.52			0.1301	0.1007	0.293	0.0316	0.0446	0.0176
Pa	91	0.561	0.492	1.69	1.77								
U	92	0.572	0.495	1.76	2.63			0.239	0.0986	0.290	0.0138	0.0191	0.0159
Np	93	0.581	0.497	1.82	2.76			0.407	0.1006	0.301	0.0142	0.0196	0.0160
Pu	94	0.580	0.496	1.88	2.88			0.606	0.1022	0.312	0.0145	0.0199	0.0161
Am	95	0.596	0.494	1.95	2.98			0.933	0.0988	0.304			0.0138
Cm	96	0.603	0.492	2.02	3.10			1.20	0.0995	0.313			0.0138
					3.25			1.40	0.1042	0.340	0.0149	0.0200	0.0163

Table 2. Photoionization cross sections at 1487 eV in units of the C 1s cross section of 13,600 barns.

Z	Total	1s1/2	2s1/2	2p1/2	2p3/2	3s1/2	3p1/2	3p3/2	3d3/2	3d5/2	4s1/2	4p1/2	4p3/2
H	1	0.0002	0.0002										
He	2	0.0082	0.0082										
Li	3	0.0576	0.0568	0.0008									
Be	4	0.202	0.1947	0.0072									
B	5	0.508	0.486	0.0220	0.0001	0.0001							
C	6	1.05	1.000	0.0477	0.0005	0.0010							
N	7	1.69	1.80	0.0867	0.0022	0.0043							
O	8	3.09	2.93	0.1405	0.0065	0.0128							
F	9	4.68	4.43	0.210	0.0161	0.0317							
Ne	10	6.70	6.30	0.296	0.0347	0.0683							
Na	11	9.14	8.52	0.422	0.0654	0.1287	0.0064						
Mg	12	12.11	11.18	0.575	0.1125	0.221	0.0285						
Al	13	1.35	0.753	0.1811	0.356	0.0535							
Si	14	1.87	0.955	0.276	0.541	0.0808	0.0011	0.0022					
P	15	2.52	1.18	0.403	0.789	0.1116	0.0047	0.0093					
S	16	3.33	1.43	0.567	1.11	0.1465	0.0124	0.0244					
Cl	17	4.31	1.69	0.775	1.51	0.1852	0.0262	0.0512					
Ar	18	5.49	1.97	1.03	2.01	0.227	0.0486	0.0947					
K	19	6.90	2.27	1.35	2.62	0.286	0.0821	0.1597			0.0069		
Ca	20	8.55	2.59	1.72	3.35	0.351	0.1229	0.239			0.0268		
Sc	21	10.39	2.91	2.17	4.21	0.411	0.221	0.429	0.0017	0.0025	0.0314		
Ti	22	12.48	3.24	2.69	5.22	0.473	0.276	0.537	0.0055	0.0081	0.0355		
V	23	14.84	3.57	3.29	6.37	0.538	0.339	0.657	0.0125	0.0184	0.0394		
Cr	24	17.43	3.91	3.98	7.69	0.596	0.400	0.773	0.0264	0.0387	0.0161		
Mn	25	20.39	4.23	4.74	9.17	0.674	0.485	0.938	0.0424	0.0622	0.0464		
Fe	26	23.61	4.57	5.60	10.82	0.745	0.569	1.10	0.0694	0.1017	0.0497		
Co	27	27.10	4.88	6.54	12.62	0.818	0.660	1.27	0.1082	0.1582	0.0529		
Ni	28	30.90	5.16	7.57	14.61	0.892	0.757	1.46	0.1619	0.236	0.0560		
Cu	29	34.90	5.46	8.66	16.73	0.957	0.848	1.63	0.240	0.349	0.0621		
Zn	30	39.22	5.76	9.80	18.92	1.04	0.968	1.86	0.330	0.480	0.0618		
Ga	31	44.09	6.07	11.09	21.40	1.13	1.10	2.11	0.442	0.643	0.0882	0.0062	0.0116
Ge	32	49.42	6.31	12.52	24.15	1.23	1.24	2.39	0.578	0.842	0.1119	0.0159	0.0377
As	33	48.73		14.07	27.19	1.32	1.39	2.68	0.741	1.08	0.1357	0.0417	0.0792
Se	34	51.18		13.66	28.90	1.43	1.55	2.98	0.934	1.36	0.1605	0.0724	0.1376
Br	35	9.91				1.53	1.72	3.31	1.16	1.68	0.1863	0.1129	0.215
Kr	36	11.34				1.64	1.89	3.55	1.42	2.06	0.213	0.1643	0.312
Rb	37	12.91				1.75	2.07	4.00	1.72	2.49	0.251	0.214	0.411
Sr	38	14.62				1.86	2.25	4.37	2.06	2.99	0.291	0.265	0.510
Y	39	16.45				1.98	2.44	4.75	2.44	3.54	0.329	0.311	0.599
Zr	40	18.44				2.10	2.64	5.14	2.87	4.17	0.367	0.357	0.689
Nb	41	20.57				2.22	2.84	5.53	3.35	4.86	0.402	0.398	0.767
Mo	42	22.90				2.34	3.04	5.94	3.88	5.62	0.440	0.445	0.860
Te	43	25.39				2.45	3.23	6.36	4.46	6.47	0.479	0.494	0.955
Ru	44	28.08				2.57	3.44	6.78	5.10	7.39	0.519	0.544	1.05
Rh	45	30.97				2.70	3.64	7.21	5.80	8.39	0.560	0.595	1.15
Pd	46	34.03				2.81	3.83	7.63	6.56	9.48	0.598	0.641	1.24
Ag	47	37.33				2.93	4.03	8.06	7.38	10.66	0.644	0.700	1.36
Cd	48	40.87				3.04	4.22	8.50	8.27	11.95	0.692	0.762	1.49

vacancy states, then only the sum of the cross-sections for the production of the mixed single vacancy states will be of relevance.

The Hartree-Slater model has been used for a number of previous photoionization calculations. These include those of Cooper⁵, Combet Farnoux⁶, Manson and Cooper⁸, and of Henry et al.⁷ Compilations using the non-relativistic version of the model have been given by McGuire⁹ and in conjunction with experimental data by Viegele¹⁰. Henke and Ebisu¹¹ have used experimental data and Viegele's calculated results to present the total absorption cross-sections for a large number of characteristic x-ray energies including the two here. The relativistic model has been used by Brysk and Zerby¹² and compilations based on it have been presented by Storm and Israel¹³, by Barfield et al.¹⁴ and by Scofield¹⁵. Barfield et al.¹⁴ present the subshell cross sections for the low Z elements in a form convenient to interpolate to a given energy. The subshell cross-sections are listed from 1 to 1500 keV in the report by Scofield. The subshell cross-sections for the two energies covered here have previously been given by Nefedov et al.¹⁶ for Z values up to 20.

Comparing the total cross-section results of the present calculation with the experimentally derived low Z values listed by Henke and Ebisu¹¹ and the cross-sections with small experimental uncertainties listed in Section III of the compilations of McMaster et al.¹⁷ shows agreement to within 5% for all except the high Z elements. For the elements for which the N shell is the major contributor, the differences rise to approximately 10%; for the photoabsorption in uranium at these energies recent experiments of Del Grande and Oliver¹⁸ show 16% differences.

The experimental results for the subshell cross-sections have thus far been too fragmentary for a clear picture of the reliability of these theoretical results. Results of the measurements in solids^{3, 16, 19, 20} have a large amount of scatter but show a general agreement with the theoretical results within something like 30%. Most of the results of Kemeny et al.²⁰ for NaF and NaCl agree well with the present values except the 3s result in chlorine which is one-half the theoretical value. The relative cross-sections for the 3s, 3p and 3d shells in krypton²¹ agree with the results of the model. Results from the Uppsala group reported by Gelius²² show systematic discrepancies for the 2s/2p and 3s/3p cross-section ratios presented per electron. For carbon their 2s/2p ratio is one-half the theoretical value and, progressing to neon it is 1.2 times the theoretical. Their experimental value of the 3s/3p ratio is one-third of the theoretical value for sulfur and 0.6 times the theoretical value for argon. Experiments of Wuilleumier and Krause²³ for neon find the cross-sections, with those for multivacancy production included, for the 2s vacancy production 0.7 times the Hartree-Slater value and for 2p 0.8 times this value. In contrast to the Uppsala group's value, their 2s/2p value is 0.8 times the theoretical value.

The inaccuracy in the Hartree-Slater model in the treatment of the photoionization from isolated atoms comes about because of the approximate manner of treating the electron-electron interactions. The problem of more accurately calculating the magnitude and the structure of the photoelectron spectrum is being pursued using

a number of different methods. Recent review articles which treat the theoretical approaches include Fano and Cooper²⁴, Pratt et al.²⁵, Fadley²⁶ and Cooper²⁷.

ACKNOWLEDGEMENT

This work was performed under the auspices of the Energy Research and Development Administration.

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