

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

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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 Slater<sup>1</sup> 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 Slater<sup>1</sup>. With the necessary modifications to treat the continuum states, the treatment follows that used previously for the calculation of the characteristic X-ray emission rates<sup>2</sup>.

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.<sup>3</sup> and that at 1254 eV by Swingle<sup>4</sup>. 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 (continued). Cross sections at 1254 eV in units of 22,200 barns.

Table with columns Z, 5s1/2, 5p1/2, 5p3/2, 5d3/2, 5d5/2, 5f5/2, 5f7/2, 6a1/2, 6p1/2, 6p3/2, 6d3/2, 6d5/2, 7s1/2. Rows include elements from In (Z=49) to Cd (Z=48).

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

Table with columns 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. Rows include elements from H (Z=1) to Cd (Z=48).

Table 2 (continued). Cross sections at 1487 eV in units of 13,600 barns.

Table with 14 columns (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) and rows for elements In to Cm.

Table 2 (continued). Cross sections at 1487 eV in units of 13,600 barns.

Table with 15 columns (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) and rows for elements In to Cm.

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 Cooper<sup>5</sup>, Combet Farnoux<sup>6</sup>, Manson and Cooper<sup>8</sup>, and of Henry et al.<sup>7</sup> Compilations using the non-relativistic version of the model have been given by McGuire<sup>9</sup> and in conjunction with experimental data by Viegele<sup>10</sup>. Henke and Ebisu<sup>11</sup> 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 Zerby<sup>12</sup> and compilations based on it have been presented by Storm and Israel<sup>13</sup>, by Barfield et al.<sup>14</sup> and by Scofield<sup>15</sup>. Barfield et al.<sup>14</sup> 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.<sup>16</sup> 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 Ebisu<sup>11</sup> and the cross-sections with small experimental uncertainties listed in Section III of the compilations of McMaster et al.<sup>17</sup> 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 Oliver<sup>18</sup> 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<sup>3, 16, 19, 20</sup> 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.<sup>20</sup> 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 krypton<sup>21</sup> agree with the results of the model. Results from the Uppsala group reported by Gelius<sup>22</sup> 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 Krause<sup>23</sup> 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 Cooper<sup>24</sup>, Pratt et al.<sup>25</sup>, Fadley<sup>26</sup> and Cooper<sup>27</sup>.

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