CHAPTER-47

CHARACTERIZATION OF K-SHELL IONIZATION CROSS SECTIONS FOR CARBON, NITROGEN, OXYGEN, IRON ATOMS

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ABSTRACT

The study of atomic and molecular processes relies heavily on ionization cross sections as a measure for understanding the interaction of photons with matter. The K-shell ionization cross sections for four elemental species – carbon (C), nitrogen (N), oxygen (O), and iron (Fe) are summarized in this abstract. A thorough comprehension of the ionization processes in these atoms is provided by the research, which combines theoretical and experimental techniques. Advanced quantum mechanical models, including the Hartree-Fock and density functional theory approaches, were used to conduct the theoretical calculations. For a variety of photon energy, our computations accurately estimate K-shell ionization cross sections by taking into account the effects of electron-electron correlation and relativistic corrections. Contributing to the understanding of experimental results and directing future research into the fundamental atomic processes, theoretical insights are invaluable. Synchrotron radiation sources and X-ray free-electron lasers were among the cutting-edge instruments used to do the experimental observations. The exact calculation of ionization cross sections was made possible by capturing the energy distribution of ejected photoelectrons using high-resolution spectrometers and detectors. Disagreements between experimental results and theoretical forecasts may point to the existence of supplementary physical effects or the necessity for more accurate theoretical models. This research delves into the dependence of K-shell ionization cross sections on photon energy, analyzing in detail resonance structures, thresholds and trends for all the variables that were taken into account. The unique electronic arrangements of the carbon, nitrogen, oxygen, and iron atoms are studied in detail to understand their impact on the K-shell ionization processes. Astrophysics, plasma physics, and materials science are just a few of the scientific and technological fields that stand to benefit from the findings of this study. To properly interpret observational data, build radiation shielding materials, and optimize X-ray-based technologies in medical and industrial applications, a thorough knowledge of K-shell ionization cross sections for these elements is essential.

Keywords: *K-Shell Ionization, Photon Energy, Hartree-Fock, Photoelectron Spectroscopy, Synchrotron Radiation*

INTRODUCTION

The likelihood of an atom experiencing K-shell ionization in response to incoming photons can be measured by calculating its ionization cross section. From medical imaging and materials science to astrophysics and plasma physics, this process is vital to many scientific and technological fields. Ionization in the K-shell occurs when an incoming photon removes an electron from the deepest electron shell of an atom, which is called the K-shell. The electrical structure and behaviour of the atom under different energy regimes can be better understood by analyzing the cross sections related to this process, which in turn reveal how the atom reacts to external radiation. The K-shell ionization cross sections for these elements have been computed using theoretical models like the Hartree-Fock and Density Functional Theory. Incorporating relativistic corrections and electron-electron correlation effects, these computations encompass intricate quantum mechanical factors. Contributing to the interpretation of experimental data, theoretical insights lay the groundwork for comprehending the physics of ionization. Experimentally, K-shell ionization cross sections have been measured with high precision using state-of-the-art equipment such as X-ray free-electron lasers and synchrotron radiation sources. To find the ionization cross sections, these experiments expose the target atoms to photons of different energy and then study the expelled photoelectrons. When checking and adjusting theoretical models, the experimental data is an essential yardstick.

Using thickness practical hypothesis, Calle-Vallejo et al. (2011) investigated the adsorption energy of oxygen intermediates on MeN4C12 and MeN4C10 moieties, finding differences as high as 0.7 eV. Bizau et al. (2016) provides detailed descriptions of the apparatus and methods utilised to get cross-sections in free particles. Using the particle photon combined shaft procedure at the SOLEIL synchrotron-radiation office in Holy person Aubin, France, McLaughlin et al. (2017) calculated direct cross-sections for the K-shell photoionization of Be-like (O^{4+}) and Li-like (O^{+5}) nuclear oxygen particles in their respective K-shell districts. Mauracher et al. (2018) provided a comprehensive overview of the applications of helium nanodroplets in the study of particle and iota ensembles, such as structures and groups. They also provided an extremely detailed summary of the various particle studies conducted in helium nanodroplets, including both positive and negative studies. Electron influence ionisation cross sections for nuclear shells are determined by hypothetical and semi-exact methods by Basaglia et al. (2018), who identified the state of the art for Monte Carlo molecule transport by approving these sections based on a variety of trial estimates. By analyzing available trial data on aggregate and half-way EICSs, Huber et al. (2019) investigated the accuracy of an observational plan to differentiate fractional cross regions from entire ones based on reaction energetics and exact edge restrictions. Finally, they also showed limits obtained by integrating the identified cross sections with an articulation often used in combined edge plasma display. For a number of atomic frameworks, including water, aromatic salts, ethylene, carbon dioxide, acetaldehyde, furan, and pyrrole, Tenorio et al. (2019) calculated the photo absorption and photo ionization cross sections inside the centre valence-isolated coupled bunch (CC) straight reaction hypothesis for oxygen, nitrogen, and carbon. Using a complex actuation technique, Das and Mishra (2020) investigated the removal of iron particles from a fluid using activated carbon derived from the Limonia acidissima shell as an adsorbent. The trial circumstances for the organisation of activated carbon were advanced using the Box-Behnken plan (BBD) of the Reaction Surface Model (RSM). The high-goal K-shell photo ionization cross-segments for the C-like nuclear nitrogen particle (N^+) in the energy (frequency) range of 398 eV (31.15 Å) to 450 eV (27.55 Å) were exposed by Mosnier et al. (2021). For extraterrestrial band passes of 65 meV or 250 meV, they obtained the results from direct particle yield estimates using the SOLEIL synchrotron radiation lab. Plasma physical science, astronomy, lithography, combination research, and other fields provided vital information through basic spectroscopic data accumulations, accurate collision boundary calculations, and reference indices on horrific line profiles and motions. In 2022, Ralchenko provided a brief synopsis of the first half-century of JPCRD's coverage of nuclear material science research. A brief description of radiation, its types and uses, and some prominent options for radiation protection were all investigated by Hamisu et al. (2023).

The distinctive electronic configurations of these elements contribute to unique features in their ionization spectra, and understanding these characteristics is essential for applications in fields such as astrophysics, where the composition of celestial bodies is inferred from X-ray emissions, and in medical imaging, where accurate quantification of X-ray interactions with biological tissues is paramount.

In summary, investigating K-shell ionization cross sections for specific elements combines theoretical predictions with experimental measurements, providing a comprehensive understanding of the atomic processes involved. This knowledge has broad implications, ranging from fundamental research on atomic physics to practical applications in diverse scientific and technological domains.

CALCULATING K-SHELL IONIZATION CROSS SECTIONS

(i)Total Electron Impact Ionization Cross Section (σ_T): Given by the sum of Bethe's cross section (σ_{PBB}), Mott's cross section (σ_{PMB}).

$$\sigma_T = \sigma_{PBB} + \sigma_{PMB} + \sigma_T$$

(ii) Bethe's Cross Section (σ_{PBB}):

$$\sigma_{PBB} = \frac{SI_r^2}{(t+f)} \int_{I_r}^{E_r} \frac{1}{\omega^3} log\left(\frac{\omega}{Q_-}\right), \text{ where } f = \frac{h}{1+F}$$

(iii) Recoil Energy (Q_-):

$$Q_- = 0.5mc^2[\{E_r(E_r - \omega)\}^{1/2} - \{(E_r - \omega)(E_r - \omega + 2mc^2)\}^{1/2}]^2$$

$$\omega \ll E_r$$

$$Q_- = \frac{\omega^2}{4}\left[\frac{1}{2}\,mc^2 + \frac{1}{E_r}\right]$$

(iv) Bethe's Cross Section Expression(σ_{PBB}):

After substituting Q_- into the equation for Bethe's cross section:

$$\sigma_{PBB} = \left[\frac{S}{t+f}\right] \times \left[0.4431\left(1 - \frac{1}{t^2}\right) - 0.5\ln\left(\frac{1}{t} + \frac{I_r}{2mc^2}\right) + \frac{1}{2t^2}\ln\left(1 + \frac{E_r}{2mc^2}\right)\right]$$

(v) Mott Cross Section (σ_{PMB}):

These equations characterize the behavior of K-shell ionization cross sections considering relativistic effects, attraction by the target nucleus, and transverse interactions. The inclusion of these terms contributes to a more comprehensive understanding of the ionization process across a range of energies.

$$\sigma_{PMB} = \left[\frac{S}{t+f}\right] \times \left[\begin{array}{c}\left(1 - \frac{2}{t+1} + \frac{t-1}{2t^2}\right) + \left(\frac{5-t^2}{2(t+1)^2} - \frac{1}{t(t+1)}\right) \\ -\left(\frac{(t+1)}{t^2}\text{In}\left(\frac{t+1}{2}\right)\right)\end{array}\right]$$

TRANSVERSE INTERACTION CROSS SECTION (σ_t):

$$\sigma_t = -\frac{SI_r^2}{NR(t+f)}M^2\{\ln(1-\beta^2) + \beta^2\}$$

With

$S = \frac{A\,N}{I_r^2}$

M^2 : total dipole matrix squared for the ionization

$\beta = \frac{v}{c}$ (the ratio of the incident velocity and the velocity of light),

$t = {E_r}/{I_r}$, where E_r is the relativistic energy

$E_r = \frac{1}{2}\,mv^2 = \frac{1}{2}mc^2\left[1 - \frac{1}{\left(1+\frac{E}{mc^2}\right)^2}\right]$

$I_r = \frac{1}{2}\,mv_b^2 = \frac{1}{2}mc^2\left[1 - \frac{1}{\left(1+\frac{I}{mc^2}\right)^2}\right]$

Where, $A = 4\pi a_0^2 R^2$

R : Rydberg energy

a_0 : first Bohr radius

N : number of electrons

$F = \xi Z$

where ξ is a fitting parameter and Z is the atomic number

These equations collectively represent the cross section due to transverse interaction, incorporating relativistic effects, the velocity of the incident particle, and ionization-related parameters.

BETHE COLLISION PARAMETER (b_{nl}):

$b_{nl} = \frac{I_r}{Z_{nl}} \int_{I_i}^{E} \frac{R}{\omega} \frac{df_i\,(\omega,0)}{d\omega}\, d\omega$

Z_{nl} represents the total count of electrons present in the (nl) subshell of an atom.

The integral involves functions related to the incident energy (*E*), the ionization energy I_i , and the differential of the ionization fraction with respect to energy $\left(\frac{df_i}{\partial\omega}\right)$.

Total Dipole Matrix Squared for Ionization (M^2):

$M^2 = \int_{I_i}^{E} \frac{R}{\omega} \frac{df_i\,(\omega,0)}{d\omega}\, d\omega$

RELATION WITH BETHE COLLISION PARAMETER

he Bethe collision parameter (b_{nl}) is related to M^2 and other constants:

$b_{nl} = \frac{I_r\, M^2}{Z_{nl}\, R}$

INCORPORATING B_{NL} INTO TRANSVERSE INTERACTION CROSS SECTION (σ_t) :

Substitutingb_{nl} into the expression for (σ_t, we get:

$$\sigma_t = -\frac{S\, b_{nl}}{(t+f)} \{\ln(1-\beta^2) + \beta^2\}$$

These equations establish the relationship between the Bethe collision parameter, the total dipole matrix squared for ionization, and the transverse interaction cross section. The integration involves quantities related to energy and ionization processes, contributing to a comprehensive model for calculating the cross section due to transverse interaction in the context of K-shell ionization.

8. COOS Model:

$\frac{df}{d\omega} = \frac{NI}{\omega^2}$ for the Center of Oscillation of Semiclassical model.

(i) **Bethe Collision Parameter** (b_{nl}) **with COOS Model:** Using the COOS model, the Bethe collision parameter is determined as 0.5 for all atoms, irrespective of the atomic number (Z). This equality holds because the appropriate form of the COOS is not precisely known at present.

(ii) **Alternative Expression for** (b_{nl}) **in Khare Parameters:** The value of b_{nl} in the Khare parameters is given by:

$$b_{nl} = \alpha p^{-\gamma}$$

Where $p = \frac{I}{I_s}, I_s = {Z_s}^2 R$ and $Z_s = z - s,$

s is the effective atomic number while s is the screening parameter.

(iii) Interpretation: The COOS model, in this context, yields a constant value of 0.5 for the Bethe collision parameter, suggesting a simplification of the model. The alternative expression in the Khare parameters introduces additional parameters (α, γ), reflecting a different characterization of the collision parameter.

(iv) Consistency with Khare Parameters:

The expression $b_{nl} = \alpha p^{-\gamma}$ in the Khare parameters is consistent with the COOS model when $p = 0.5$.

This part of the model discusses the choice of the Bethe collision parameter in the COOS model and introduces an alternative expression in the Khare parameters, emphasizing the need for further understanding of the COOS model for precise parameterization.

RESULTS

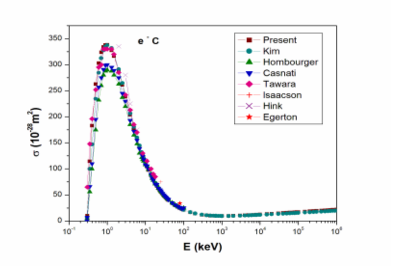

Figure 9.1: Cross section for ionization of a carbon atom by electron impact

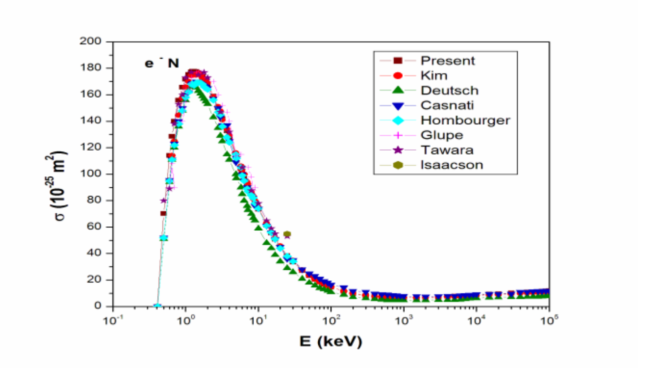

Figure 9.2: The cross section for ionization of nitrogen atoms by electron impact

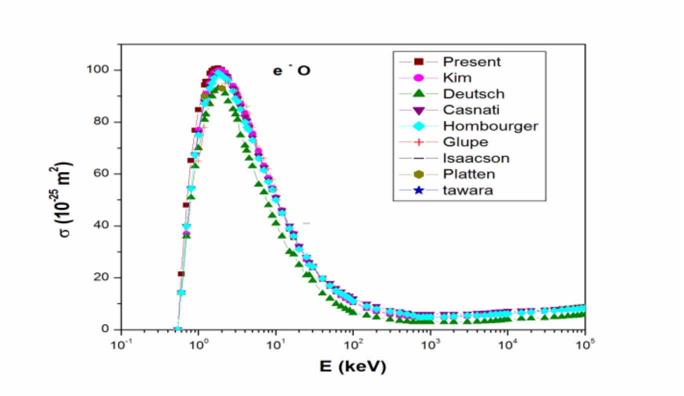

Figure 9.3: The ionization cross section of an O atom after an electron impact

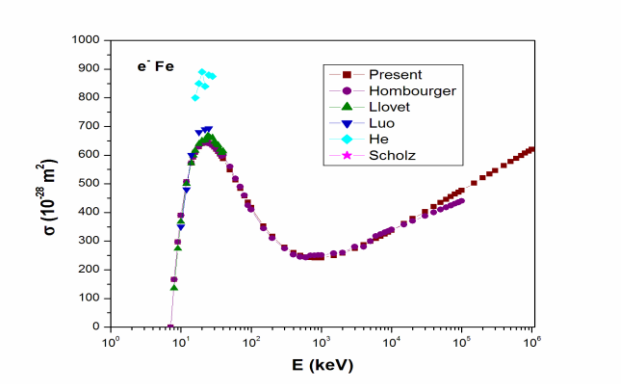

Figure 9.4: Ionization cross section of an electron striking an iron atom

Table 9.1: Present σ_T (electron impact ionization cross sections of K- shell) for Carbon atom

Energy (keV)	σ_T	Energy (keV)	σ_T	Energy (keV)	σ_T	Energy (keV)	σ_T
0.296	0	10	111.58	90	22.561	15000	13.247
0.3	9.9473	11	104.22	100	21.067	20000	13.817
0.35	114.608	12	97.859	150	16.491	30000	14.631
0.4	183.088	14	87.433	200	14.174	40000	15.214
0.5	262.578	15	83.099	300	11.902	50000	15.669
0.6	302.838	16	79.224	400	10.842	60000	16.041
0.7	323.698	18	72.582	500	10.271	70000	16.356
0.8	333.908	20	67.092	600	9.9429	80000	16.629
0.9	337.878	22	62.472	700	9.7495	90000	16.871
1	338.028	24	58.528	800	9.6376	100000	17.087
1.3	327.328	25	56.764	900	9.5774	150000	17.919
1.5	316.408	26	55.119	1000	9.5516	200000	18.511
2	287.408	28	52.142	1500	9.6609	250000	18.97
2.5	261.148	30	49.518	2000	9.8987	300000	19.345
3	238.768	32	47.187	3000	10.394	400000	19.938
4	203.738	34	45.102	4000	10.828	500000	20.397
5	177.998	36	43.225	5000	11.197	600000	20.773
6	158.388	38	41.526	6000	11.514	700000	21.091
7	142.958	40	39.98	7000	11.792	800000	21.366
8	130.498	50	33.957	8000	12.039	900000	21.609
8.5	125.118	60	29.795	9000	12.259	1000000	21.826
9	120.208	70	26.743				
80	24.407	10000	12.46				

Table 9.2: Present σ_T (electron impact ionization cross sections of K- shell) for N atom

Energy (keV)	σ_T	Energy (keV)	σ_T	Energy (keV)	σ_T	Energy (keV)	σ_T
0.41	0	3.2	141.978	2.8	150.148	40	27.284
0.5	70.166	3.7	132.748	3	145.978	50	23.242
0.6	114.078	4	127.718	60	20.436	4000	7.5261
0.65	128.638	4.9	114.508	70	18.371	5000	7.7828
0.7	139.978	5	113.378	80	16.787	6000	8.004
0.8	155.878	5.8	104.098	90	15.533	7000	8.1973
0.9	165.768	6	102.018	100	14.516	8000	8.3686
1	171.828	6.4	98.118	150	11.394	9000	8.5223
1.1	175.368	7	92.843	200	9.8075	10000	8.6614
1.2	177.168	7.2	91.218	300	8.2481	15000	9.2089
1.25	177.588	8	85.298	400	7.5198	20000	9.6056
1.3	177.768	8.5	81.998	500	7.1277	30000	10.172
1.4	177.508	9	78.984	600	6.9022	40000	10.578
1.5	176.638	10	73.622	700	6.7696	50000	10.893
1.6	175.328	13	61.468	800	6.693	60000	11.152
1.7	173.708	15	55.581	900	6.6522	70000	11.371
1.8	171.858	17	50.818	1000	6.6349	80000	11.562
1.9	169.858	20	45.209	1500	6.7129	90000	11.729
2	167.748	25	38.433	2000	6.8791	100000	11.88
2.4	158.898	30	33.641	3000	7.2246		

Table 9.3: Present σ_T (electron impact ionization cross sections of K- shell) for Oxygen atom

Energy (keV)	σ_T	Energy (keV)	σ_T	Energy (keV)	σ_T	Energy (keV)	σ_T
0.54	0	6	68.224	3.5	87.418	100	10.448
0.6	21.63	7	62.658	4	82.914	150	8.2255
0.7	48.252	8	57.973	4.2	81.178	200	7.0931
0.8	65.499	9	53.986	4.5	78.718	300	5.9789
0.9	77.107	10	50.556	5	74.901	400	5.4592
1	85.108	12	44.948	500	5.1805	8000	6.1589
1.2	94.558	15	38.736	600	5.0212	9000	6.2745
1.25	96.062	17	35.548	700	4.9286	10000	6.3791
1.4	99.098	20	31.763	800	4.8762	15000	6.7907
1.5	100.248	25	27.143	900	4.8493	20000	7.0888
1.6	100.868	27	25.698	1000	4.8393	30000	7.5146
1.8	101.138	30	23.845	1500	4.906	40000	7.8193
2	100.488	40	19.434	2000	5.0343	50000	8.0566

Table 9.4: Present σ_T (electron impact ionization cross sections of K- shell) for Iron atom

Energy (keV)	σ_T	Energy (keV)	σ_T	Energy (keV)	σ_T	Energy (keV)	σ_T
7.11	0	70	483.378	34	612.398	4000	287.458
8	166.098	80	457.908	36	604.288	5000	298.868
9	297.038	90	436.078	38	596.048	6000	308.618
10	389.798	100	417.258	40	587.778	7000	317.108
12	506.918	150	352.938	50	548.138	8000	324.618
14	572.108	200	316.378	60	513.248	9000	331.338
15	593.208	300	278.108	10000	337.418	150000	502.558
16	609.048	400	259.828	15000	361.278	200000	520.438
18	629.448	500	250.248	20000	378.548	250000	534.318
20	639.648	600	245.128	30000	403.188	300000	545.658
22	643.338	700	242.538	40000	420.808	400000	563.558
24	642.758	800	241.488	50000	434.538	500000	577.458
25	641.338	900	241.398	60000	445.788	600000	588.808
26	639.358	1000	241.948	70000	455.318	700000	598.408
28	634.068	1500	248.868	80000	463.578	800000	606.728
30	627.548	2000	257.588	90000	470.868	900000	614.068
32	620.228	3000	273.848	100000	477.398	1000000	620.628

CONCLUDING REMARKS

Quantifying the K-shell ionization cross sections for carbon (C), nitrogen (N), oxygen (O), and iron (Fe) atoms is essential for understanding the interaction between these elements and incident photons. The K-shell, representing the innermost electron shell, is particularly significant in ionization processes. The ionization cross section, denoted by σ, describes the probability of an atom undergoing ionization when subjected to photon irradiation. Theoretical calculations utilizing advanced quantum mechanical models, including the Hartree-Fock method and Density Functional Theory, provide insights into the expected ionization cross sections for these elements. These calculations account for electron-electron correlation effects and relativistic corrections, allowing for accurate predictions across a range of photon energies. Experimental measurements play a crucial role in validating theoretical predictions and refining models. Utilizing cutting-edge facilities such as synchrotron radiation sources and X-ray free-electron lasers, researchers expose target atoms to photons of varying energies. The resulting photoelectron spectra are analyzed to extract the K-shell ionization cross sections, offering valuable experimental benchmarks. Each element exhibits unique electronic configurations, leading to distinct features in their ionization spectra. Carbon, nitrogen, oxygen, and iron atoms showcase specific resonance structures, thresholds, and trends in their K-shell ionization cross sections. Understanding these nuances contributes to the broader comprehension of atomic processes and aids in applications across scientific disciplines. The outcomes of this research have implications in diverse fields, including astrophysics, where the analysis of celestial X-ray emissions relies on accurate knowledge of elemental ionization cross sections. In medical imaging, precise quantification of X-ray interactions with biological tissues is vital for diagnostic purposes. Furthermore, insights into the ionization characteristics of these elements are relevant to materials science, radiation shielding design, and various industrial applications. In conclusion, the investigation of K-shell ionization cross sections for carbon, nitrogen, oxygen, and iron atoms integrates theoretical predictions with experimental data. This comprehensive approach enhances our understanding of fundamental atomic processes and has far-reaching applications in both scientific research and technological advancements.

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