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RESEARCH ARTICLE

Refining the Effective Atomic Number of Copper Compounds: A High-Precision Analysis via Rayleigh-to-Compton Scattering Intensity Ratios

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ABSTRACT

This study presents a comprehensive investigation into the effective atomic numbers (Z_{eff}) and electron densities (N_{eff}) of various copper compounds using the Rayleigh-to-Compton (R/C) scattering ratio method. Measurements were performed using a high-resolution HPGe detector and a ^{241}Am radioisotope source emitting 59.54 keV gamma rays. The experimental R/C ratios were utilized to derive Z_{eff} values, which were then compared with theoretical data obtained via WinXCOM. A significant correlation was observed between the chemical environment of the copper compounds and their scattering intensities. One of the main conclusions that can be drawn from the experimental results is how accurately the effective atomic number is determined using data obtained from coherent and Compton scattering. As proof of this, it is clearly seen that the Compton and coherent scattering data obtained from the copper sulfate and copper iodide samples examined during the experiment are highly sensitive to the effective atomic number of the sample used and have a significant effect on spectral analyses. In the experimental results, which also proved this situation experimentally, it is clearly seen that Compton scattering is dominant in samples with low effective atomic numbers, and conversely, coherent scattering becomes dominant in environments with high effective atomic numbers. Thus, our study, with its meaningful results obtained from theoretical calculations and experimental data, has proven that the effective atomic number can be determined in complex chemical structures using the R/C ratio, as we used in our experiments.

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1. Introduction

In today's electronic devices and technological applications, copper and certain important copper compounds, preferred due to their atomic structures, form the basis of research and development studies. Copper and its oxide structures play a significant role in superconductivity studies observed at high temperatures and in some critical chemical engineering processes (B. Singh et al., 2010). Furthermore, in semiconductor physics and electronic device development, copper and industrially important copper compounds are preferred due to their high electron-carrying capacity. In addition, the behavior of electronic and industrial devices made from copper compounds in space environments under high radiation conditions has been a subject of interest, and research has been developed in this area. As mentioned, determining the

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shielding or structural change properties of copper and its compounds under radiation and using them in the improvement of developed systems is both a necessity and a requirement for gaining practicality.

The physical response of these compounds to gamma-ray exposure is primarily dictated by their effective atomic number (Z_{eff}). This parameter serves as a crucial bridge between macroscopic material behavior and microscopic interaction cross-sections. Copper is described as an essential transition metal that is frequently used in fundamental sciences, industry, and electronics applications (Kumar et al., 2007). However, some significant differences from its general behavior are observed when copper bonds with different oxide structures and complex ligand structures (such as sulfates). Its behavior changes significantly when bonded with ligands. In fact, these structure shifting create complex electronic structures that cannot be described by standard atomic tables and require explanation. Consequently, a precise investigation into the Z_{eff} of copper compounds offers a unique window into the electronic density redistributions that occur during chemical bonding.

Applications of radiation physics and various studies conducted in this field in recent years clearly demonstrate the interest in non-destructive testing techniques. Examining these studies reveals that the mass absorption method has become a standardized technique. While traditional and standardized techniques are frequently used, efforts to minimize the direct effects encountered in calculations using standard methods by developing alternative methods are evident in literature. The Rayleigh-Compton (R/C) technique is one of these new methods and is a good example of improved experimental methods. Furthermore, this technique eliminates the fluctuations that are caused by source density and sample geometry, which are discrepancies observed in data obtained using traditional absorption techniques.

In this study, we have used different designed experimental setup compared to other researchers that includes lower-energy (59.54 keV) radiation source for irradiation. In addition, this setup includes a high-resolution semiconductor HPGe detector have used for collecting scattered photons. For atomically environment, the interaction between Rayleigh to Compton scattering is highly sensitive at lower radiation source energies. For this purpose, we have set the scattering angle at 167^0 to maximize the energy seperation at Compton and coherent peaks. This allows for a more precise detection of "chemical effects" on Z_{eff}, providing a level of detail that surpasses the generalized approximations found in current radiation interaction databases.

Many technological and industrial applications, such as medical physics and nuclear engineering, are based on creating the most effective radiation shielding design by taking data collected from the interaction of all types of radiation, especially gamma radiation, with matter (Hubbell, 1982; Knoll, 2010). A wide understanding of these procedures requires precise knowledge of Z_{eff}, a parameter first conceptualized to treat composite materials as if they were a single element (Hine, 1952). While the atomic number Z is constant for pure elements, for compounds, Z_{eff} varies depending on the incident photon energy and the specific interaction process involved (Jackson & Hawkes, 1981).

In recent decades, Z_{eff} determination has mostly relied on the total mass attenuation coefficient (μ/ρ) method. However, studies conducted using the mass absorption technique facing significant technical barriers in terms of homogeneity and thickness accuracy of the samples used in the experiment, as noted by various researchers (Han & Demir, 2009; M. P. Singh et al., 2010). Nevertheless, the R/C scattering density ratio has emerged as a robust alternative because it minimizes the source fluctuations and systematic errors related to sample density encountered in other techniques (Duvauchelle et al., 1999; Tursucu et al., 2013). Despite the importance of copper compounds in modern electronics (Edelstein et al., 1997), experimental data on their Z_{eff} especially regarding chemical environment effects remain scarce. Most available data still rely on theoretical structures like WinXCOM (Gerward et al., 2001), which can be able to overlook the fine electronic shifts at the molecular level. Building on our previous work with rare earth oxides (Turşucu et al., 2023), this study aims to fill this gap by providing a high-precision analysis of copper compounds using the refined R/C scattering technique (Jangir et al., 2026).

With this goal in mind, we focused our analysis on a specific set of copper-based materials. These compounds were not chosen at random; they span a broad range of chemical environments and are strategically important in modern technology, where understanding their response to radiation is a practical necessity. Copper-based materials that are used in experimental studies have some specifications and are investigated in three section. In first section, intermetallic and semiconductor advance compounds mentioned. Cu_5Si (Copper Silicide) intermetallic compound is critical in silicon-based microelectronics. The primary purpose of this compound is to form ohmic contacts, thereby creating diffusion barriers. The comprehension of the radiation's effect on this circuit contact element is also crucial. We did these tests with less radiation to do this. We will learn how it reacts to more radiation by using this information. Cu_3N (Copper Nitride) is metastable semiconductor that has gained extensive interest for optical write-once-read-many (WORM) data storage and as a high-performance electrode material in rechargeable batteries. In nanotechnology, this compound is called a smart material (Demir & Turşucu, 2013). It can stay stable in high temperatures and break down when hit by lasers that are very precise. In second section, chalcogenides and tellurides are mentioned. CuS (Copper Sulfide): Beyond its natural occurrence, CuS is a vital p-type semiconductor used in photo thermal therapy and as a secondary component in thin-film solar cells (CIGS). $CuTe_2$ (Copper Telluride): Known for its complex phase transitions, it is a key material in thermoelectric devices which convert waste heat into electricity. Its high Z components (Tellurium) provide a significant contrast in our Z_{eff} scattering analysis. $CuSe_45(H_2O)$ and H_4CuO_5Se: Selenium is a kind of metalloid that allows for the analysis of diverse effective atomic number patterns during the transition from metallic to covalent bonding. These selenium-based compounds are essential in glass manufacturing and trace minerals in specialized chemical synthesis. We have mentioned the halides and ionic matrices copper compounds in last section. One of these ionic matrices compound is CuI (Copper Iodide) that is a transparent p-type conductor and mandatory component in perovskite solar cells and organic light-emitting diodes (OLEDs). It is notable for its elevated iodine concentration in assessing the R/C sensitivity of substantial atomic compounds utilized in experiments. The other one is $CuSO_4$ (Copper Sulfate) that is a foundational material for electroplating and agricultural chemistry, serving as our benchmark for ionic crystal structures in radiation interaction studies.

In this study, we have studied the copper and its industrial, technological significance compounds. In addition, we calculated certain atomic parameters both theoretical and experimental associated with them. Finally, the experimentally determined effective atomic numbers have been compared with the values obtained in theoretical calculations, and the chemical effects outcomes on the calculated parameters and the discussions were presented together.

2. Experimental Details

2.1. Instrumentation and Geometry

The experimental setup and the following analysis, calculations, and measurements of the obtained data were carried out by using a specifically engineered for high-resolution spectroscopy investigations at scattering geometry. At the heart of the setup is a 5 Ci ^{241}Am annular radioactive source, which provides a steady, monoenergetic 59.54 keV gamma-ray flux. Annular structured radioactive source was selected deliberately to avoid unexpected background counts and ensure the monochromatic spectrum that is collected by highly sensitive detectors. Also, this selection was protecting the detector from directly counting's originating from source.

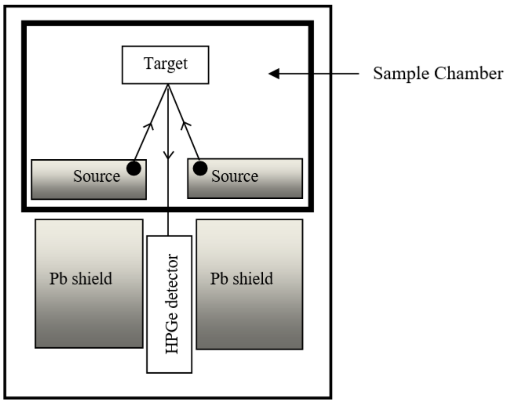

Figure 1. Experimental setup.

The dimensions of the sample holder are presented in Figures 1 and 2. The scattered radiation was measured using a high-purity germanium (HPGe) semiconductor detector. In this experiment, an angle of 167° was selected because at this angle, the difference between the Compton and coherent peaks becomes distinct. To prevent any radiation interference or contamination, lead shields were placed around the sample holder.

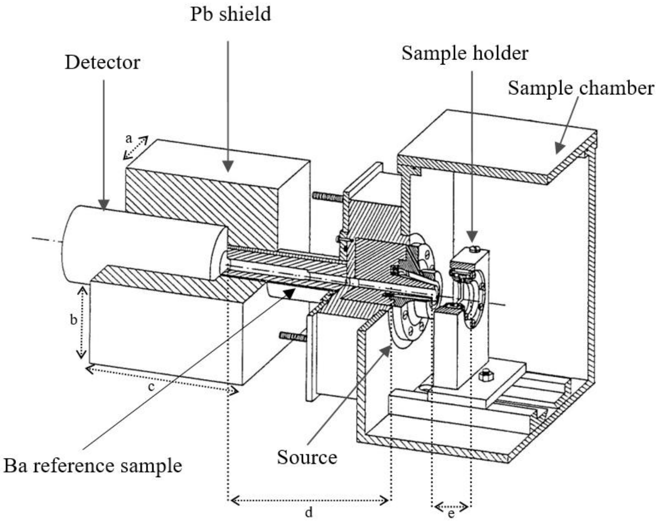

Figure 2. Sample chamber (a=6.5 cm, b=6.3 cm, c=13.5 cm, d=11 cm, e=5 cm).

2.2. Sample Preparation and Data Acquisition

In this experiment, our main emphasis was on the study of pure copper and some significant compounds of copper. For each sample taken, the laboratory-prepared samples were in the form of cylinders. In order to achieve homogeneity of samples, the powder samples were first ground in the mortar to become finely ground. Afterward, these samples were compressed into cylinders through the hydraulic press.

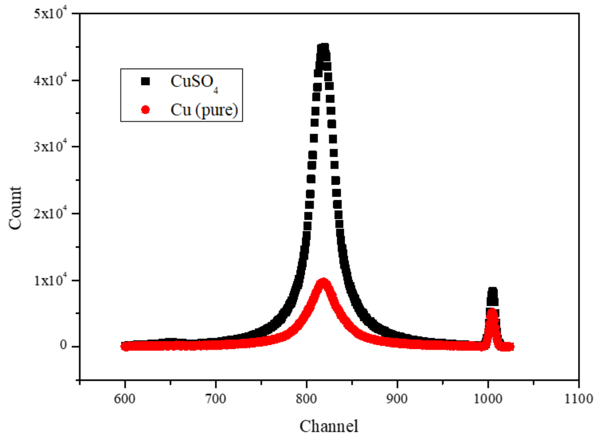

Figure 3. Comparison of scattering spectra for pure Cu and CuSO4 (Experimental pulse height spectra of pure metallic Copper ($Z = 29$) and Copper Sulfate ($CuSO_4, Z_{eff} \cong 21.6$) recorded at a scattering angle of 167°. The plot highlights the transition in scattering intensities as a function of the effective atomic environment.).

The high-resolution detector together with the multi-channel analyzer was used to collect the photons so that spectral data can be achieved (Turhan et al., 2020). Time duration in analysis was set up in such a way that the total number of counts in each spectrum will be 10.000 counts per peak. In this way, we could achieve meaningful and computational data from Rayleigh and Compton spectra. Typical spectra like those presented in Figures 3 and 4 show the difference between coherent and incoherent parts of our selected geometry.

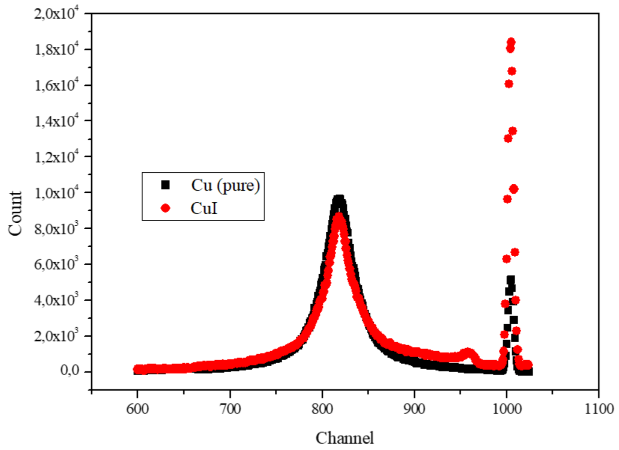

Figure 4. Comparison of scattering spectra for pure Cu and CuI (Pulse height spectra for pure Copper ($Z = 29$) and Copper Iodide ($CuI, Z_{eff} \cong 48.8$). The comparison demonstrates the spectral dominance of high$-Z$ constituents within a copper-based molecular framework.).

2.3. Calibration and Correction Procedures

Accurate Z_{eff} determination requires more than just raw counts; it demands careful correction of the experimental data. It is necessary to consider the following parameters, which include the efficiency of detector photopeak's, the most important of which is considered to be (Zhong et al., 2023). The photopeak efficiency of the HPGe detector (ε) was measured quite accurately according to the calibration sources and pure elements, as shown in the efficiency diagram in Fig. 5. The second parameter is the influence of the attenuation factor. Attenuation caused by the layer of air separating the detector from the sample and by the sample's own absorption was considered.

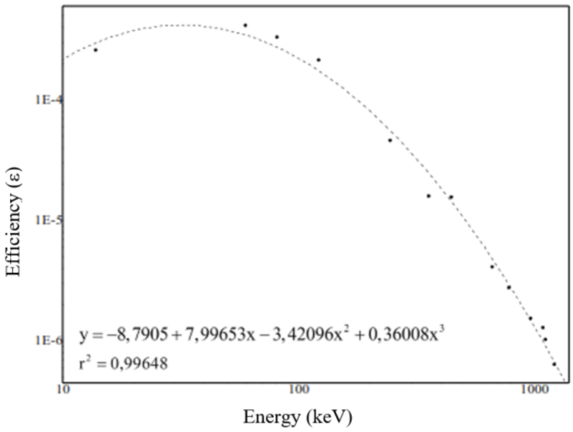

Figure 5. The photopeak efficiency curve for HPGe detector.

Self-absorption correction was handled according to the established transmission-based methodology to ensure that the final R/C ratios reflect the true scattering probabilities of the material. And the last one is the calibration curve that was used in this experiment. A primary calibration was performed using elements ($4 \leq Z \leq 82$). The resulting fit curve (Figure 6) serves as our reference for interpolating the Z_{eff} value of copper compounds.

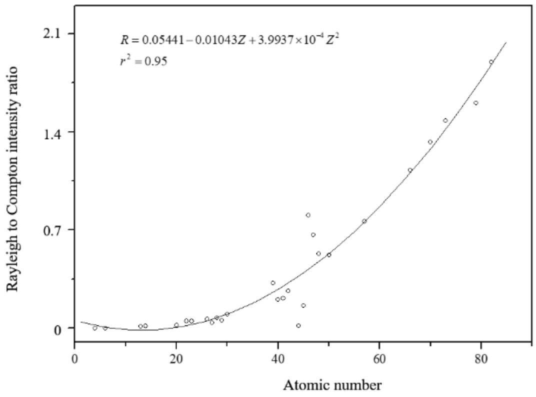

Figure 6. Rayleigh to Compton scattered intensity as a function of atomic number.

3. Theoretical Background

In recent years, the characterization of material properties through the interaction of ionizing radiation has gained significant importance. Specifically, the determination of effective atomic numbers (Z_{eff}) and electron densities (N_{eff}) for both pure elements and complex compounds depend on the certain measurement of scattering intensity ratios. The above procedure is grounded on the fact that the process of coherent and incoherent scatterings is real physically and exists in the sample itself.

3.1. Coherent (Rayleigh) Scattering

Rayleigh scattering refers to the physical process whereby the incident photon undergoes an elastic collision with the electrons bound in the sample. In this process, both the energy and the wavelength of the photon are conserved, while only the direction changes. The differential cross-section for this elastic process is expressed as:

$$\frac{d\sigma_R}{d\Omega} = \frac{r_0^2}{2}(1 + cos^2\theta)|F(q,Z)|^2 \tag{1}$$

In this expression, $F(q,Z)$ denotes the atomic form factor, which accounts for the distribution of electrons, while q, r_e, and θ represent the momentum transfer, classical electron radius, and scattering angle, respectively.

3.2. Incoherent (Compton) Scattering

The process of Compton scattering consists of an inelastic scattering process of high energy photons on atomic electrons unlike other processes of elastic scattering. The Compton scattering phenomenon is used as empirical evidence that the particles of radiation have properties of momentum transfer and decrease in frequency (Cinan & Yılmaz, 2021). The differential cross-section for such inelastic scattering is governed by the Klein-Nishina formulation:

$$(\frac{d\sigma}{d\Omega})_{KN} = \frac{1}{2} r_0^2 \left(\frac{E}{E_0}\right)^2 (\frac{E_0}{E} + \frac{E}{E_0} - sin^2\theta) \tag{2}$$

Where E_0 and E correspond to the incident and scattered photon energies. The degree of momentum transfer is significantly influenced by the incoherent scattering function, $S(q,Z)$. In high momentum transfer conditions, $S(q,Z)$ approaches the total number of atomic electrons (Z), whereas it decreases as the transfer approaches zero.

3.3. The R/C Ratio and Effective Atomic Number

This study was based on a fundamental principle that namely Rayleigh to Compton scattering cross-section ratio. This principle (R/C) ensures a unique spectral signature that is strictly related to the atomic environment of the target material investigated. The atomic Compton scattering cross-section ($\sigma_{inc,a}$), occurring from bound electrons, is defined as:

$$R = \left(\frac{d\sigma}{d\Omega}\right)_R \Big/ \left(\frac{d\sigma}{d\Omega}\right)_{aC} \propto \frac{|F(q,Z)|^2}{S(q,Z)} \tag{3}$$

$$(\frac{d\sigma}{d\Omega})_{aC} = S(q,Z)(\frac{d\sigma}{d\Omega})_{KN} \tag{4}$$

The parameterization of $F(q,Z)$ and $S(q,Z)$ is based on the comprehensive data provided by Hubbell (1982). The effective atomic number, Z_{eff}, is derived from the weighted atomic percentages of the sample constituents. This parameter directly reflects the electronic landscape of the target and is calculated through the following summation:

$$R = \left(\frac{d\sigma}{d\Omega}\right)_R \Big/ \left(\frac{d\sigma}{d\Omega}\right)_{aC} \propto \frac{\sum_{j=1}^{n} a_j^{at}|F(q,Z_j)|^2}{\sum_{j=1}^{n} a_j^{at} S(q,Z_j)} \tag{5}$$

$$a_j^{at} = \frac{(W_j/A_j)}{\sum_j (W_j/A_j)} \tag{6}$$

Where W_j represents the fractional weight and A_j represents the atomic mass of the jth element within the molecular structure.

4. Results and Discussion

The experimental R/C ratios, effective atomic numbers (Z_{eff}), and electron densities(N_{eff}) determined for the selected copper compounds are summarized in Table 1. To validate the experimental findings, theoretical Z_{eff} values were calculated using the WinXCOM database, and a high degree of correlation was observed across the studied energy range.

Table 1. Rayleigh to Compton scattered intensity ratio, experimental and theoretical effective atomic numbers of copper compounds.

Copper Compounds	**Rayleigh to Compton intensity ratio**	**Effective Atomic Number Experimental**	**Other Experimental**	**Theoretical**	**Effective Electron Density (Theoretical) (*electrons/g*)**
CuSO$_4$	0.0294±0.002	20.995±0.756	--	21.6	8.147E+22
CuS	0.0731±0.002	27.045±0.741	--	26.4	1.662E+23
Cu$_5$Si	0.1023±0.002	30.529±0.807	--	28.2	4.910E+22
CuI	0.4366±0.002	48.791±0.941	--	47.3	1.495E+23
CuSe$_4$.5(H$_2$O)	0.0493±0.003	23.877±0.983	--	25.8	2.853E+22
H$_4$CuO$_5$Se	0.1253±0.002	32.993±0.864	--	24.9	6.620E+22
CuTe$_2$	0.3922±0.002	47.941±0.798	--	49.8	9.413E+22
Cu$_3$N	0.0823±0.002	28.194±0852	--	24.4	7.185E+22

The sensitivity of scattering cross-sections to the chemical environment is visually demonstrated in Figures 3 and 4. Figure 3 compares the pulse height spectra of pure Copper (Z=29) and $CuSO_4$ ($Z_{eff} \cong 21.6$). As expected from the Z^n dependence of elastic scattering, the coherent (Rayleigh) peak of pure copper is significantly more intense than that of the sulfate compound. This reduction in Z_{eff} in $CuSO_4$ leads to a relative increase in the Compton profile, confirming that inelastic scattering becomes more prominent in lower-Z molecular environments.

In contrast, Figure 4 illustrates the effect of a high-Z constituent by comparing pure Copper with Copper Iodide (CuI, $Z_{eff} \cong 48.8$). The presence of Iodine ($Z = 53$) results in a dramatic enhancement of the Rayleigh peak, which nearly triples the intensity observed in metallic copper. This sharp contrast provides a robust experimental verification of the R/C method's ability to detect subtle changes in the effective atomic charge of complex materials.

The slight discrepancies observed in some compounds, such as H_4CuO_5Se, between experimental and theoretical Z_{eff} values can be attributed to the influence of molecular bonding effects and the local electronic environment, which are not fully accounted for in the independent atom model (IAM) used by WinXCOM. Overall, the consistent agreement between the measured R/C ratios and the theoretical expectations reinforce the reliability of using HPGe-based gamma-ray spectrometry for material characterization.

5. Conclusion

For the analysis of Cu based high electrical value materials, the present study has been focused on the determination of effective atomic number and effective electron density of these compounds via Rayleigh to Compton scattering ratio technique. The employment of very sensitive HPGe detector helped us obtain pronounced peaks corresponding to Rayleigh and Compton effects.

The main focus of this research work lies in demonstrating the results of the interactions of the radiation through effective atomic number of composite materials. Moreover, some values of effective atomic number of certain copper compounds obtained here constitute previously unknown data, thereby providing significant input to current literature. It is clear that the application of R/C ratio method can be considered useful in radiation protection, materials science, and medicine.

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Conflict of Interest

The authors have no conflict of interest to declare.

Disclosure of Generative AI Use

No generative artificial intelligence tools were used in the preparation of this article.

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