

**THEORETICAL CALCULATIONS OF RAYLEIGH SCATTERING CROSS SECTIONS
FOR ELEMENTS RANGE $1 \leq Z \leq 92$** **Gurjot Singh**

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ABSTRACT

The present work focuses on theoretical calculations of Rayleigh scattering cross sections for elements in range $1 \leq Z \leq 92$. It is decided to calculate the theoretical Rayleigh scattering cross sections using Form Factor approach and state of the art S-Matrix approach at incident photon energies in X-ray energy region. It is also decided to develop a proper method to calculate the theoretical values at incident energies near the subshell binding energies. In the experimental measurements various radioisotopes like ^{55}Fe , ^{109}Cd , ^{241}Am are used as the source of x-ray photons by researchers mostly. Some also employed the X-ray tube setups with secondary excitation mode. In the present work, a sincere review has been done for the theoretically and experimentally evaluated values of Rayleigh scattering cross sections. The theoretical values for some of the references are reproduced using the same approaches and the issues regarding some deviations observed are addressed.

Keywords: Rayleigh scattering, X-rays, Form Factor, S-matrix, Anomalous scattering factor

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1. Introduction

The interaction of photons with matter atoms is very important to understand various techniques for industry and medical purpose. The main processes involved are Rayleigh scattering, Compton scattering, pair production and photoelectric absorption. The interactions cross section value of these processes used in broad range of applications in fields of science are contributions of both theoretical and experimental efforts. A photon has a behavior like a particle having a zero mass zero charge and travel at a speed of light. When a photon interact with material it transfer whole of its energy to the interacting particle in material atom. The excited particle now can go through an interaction with another particle or it may lose energy in the form of a photon. The interactions of photons with matter has been widely studied over the past several decades in view of its importance in various fields of science. In the following chapter the physics of the interaction of photons with atoms is explained.

2. Theoretical and Experimental aspects

The curiosity has increased from last decades about the scattering cross sections, where the dominant process is elastic scattering, termed as Rayleigh scattering in X-ray energy region. In Rayleigh

scattering process, the incident photon imparts to the interacting electron some energy in the form of acceleration by the electromagnetic field associated with it. After interaction the photon emits photon having the same energy as the incident photon, means there is no net energy transfer from the photon to electron, resulting a phase relationship between the incident and scattered photons. Due to this coherence, the Rayleigh scattering process is called coherent scattering. Theoretically, two major approaches are developed to characterise the scattering: (i) Form-factor formalism, (ii) S-Matrix approach.

These approaches are given as follows.

(a) Form Factor formalism

J.J. Thomson gave a general formula for the scattering of unpolarised photons from the free electrons giving differential scattering cross section as

$$\frac{d\sigma_T}{d\Omega} = \frac{1}{2} r_o^2 (1 + \cos^2 \theta) \quad (1)$$

where, θ is the scattering angle through which the propagation direction of the incident photons changes and r_o is the classical radius of the free electron. For extended charge distributions, it is modified by including atomic form factor for a spherical charge distribution as given by

$$f(q) = 4\pi \int_0^\infty \rho(r) \frac{\sin(qr)}{qr} r^2 dr \quad (2)$$

where, $f(q)$ is the form factor, $\rho(r)$ is electron density, $\hbar q$ is momentum transferred to the atom during scattering. The $\rho(r)$ may be calculated using atomic ground state function as,

$$\rho(r) = \sum_{n=1}^Z |\psi_n(r)|^2 \quad (3)$$

Now if we know the number of electrons in an atom = Z , so each of the electron will be contributing totally as,

$$4\pi \int_0^\infty \rho(r) r^2 dr = Z \quad (4)$$

Using Thomson scattering formula, the scattering cross section is given as

$$\left(\frac{d\sigma}{d\Omega}\right)_{el} = \left(\frac{d\sigma}{d\Omega}\right)_T |f(q)|^2 \quad (5)$$

The better results of the scattering cross section are found using form factor approximation for the incident photons having energy well above the K -shell threshold of the target atom.

Franz [1] considered the effect of electron binding energy and incorporated the correction for the

same, the resulting form factor is called modified form factor (MF) given as

$$g(q) = 4\pi \int_0^{\infty} \rho(r) \frac{\sin(qr)}{qr} \frac{mc^2}{E_i - V(r)} r^2 dr \quad (6)$$

where, $\rho(r)$ is the charge density distribution for i th electron, $V(r)$ is the atomic potential and E_i is the binding energy of the i th electron. The values for the electrons present in individual levels are calculated and added to obtain $g(q)$. The resulting differential scattering cross section for the unpolarized photons is given by

$$\left(\frac{d\sigma}{d\Omega} \right)_{MF} = \frac{d\sigma_T}{d\Omega} |g(q)|^2 \quad (7)$$

Data tables of the Modified form factor values for the elements with $1 \leq Z \leq 100$ and momentum transfer $0 \leq q \leq 100 \text{ \AA}^{-1}$ is available [2]. This approximation provides cross section values for the incident energies well above the ionisation threshold and failed to obtain cross section values for the incident energies approaching the ionisation threshold from below and above or at large momentum transfers. To overcome the problem, the anomalous scattering factor is incorporated. The ASF's were obtained using the dispersion relation between the real and imaginary parts of the scattering amplitude at forward angles and the imaginary part is related to the photo absorption cross section by the optical theorem. The real part represents the intimacy of the incident photon energy to the binding energy of participating electron and imaginary part arise from the enhanced absorption of the incident photon in vicinity of the resonance level.

(b) S-Matrix approach

The scattering matrix (S-matrix) is an operator, which is connecting the final state of a time dependent system to its initial state. For Rayleigh scattering, the matrix element $S = \langle N | S | P \rangle$ signifies the amplitude of a particular stationary state $| P \rangle$ which would evolve by undergoing scattering from the initial state.

All considerable partial waves and multipoles are incorporated in Rayleigh scattering of a photon by the electron in the presence of potential. These calculations provide better results for the low momentum transfer as well as for large momentum transfers. The S-matrix approach correctly estimates the angular distribution shown by Rayleigh scattering at low as well as high incident photon energy. The calculations of scattering cross section values using S-matrix approach are computer intensive for high incident photon energies and high Z elements. This is because more atomic shells are involved in high Z elements and more partial wave and higher multipoles are required for high incident photon energies. Tabulated values of Rayleigh scattering cross-section [3] are available for almost all the elements at seven selected photon energies of experimentalist's choice in 65 angular steps in the range $0 \leq \theta \leq 180^\circ$. Therefore, the best possible method for the theoretical evaluation of scattering cross section is based on S-matrix calculations.

3. Literature review

The experimental researchers have been performing the investigations about the cross-sections and confirmed the outcomes by comparing with the theoretically calculated data. The experiments were performed using two types of excitation sources, having individual pro and cons. Some researchers used X-ray tube as the primary excitation source, which excites the target emitting the required photon energies. The continuous energy spectrum from the X-ray tube was filtered using selective absorbers, so that required energy can be available for the secondary excitation. In this case to incorporate the self-absorption correction in secondary excitation source becomes complex due to large background and continues energy range. The major benefit is large count rate. On the other hand, the use of radioisotope source simplifies the things due to presence of monochromatic photon beam and easy calculation of self-absorption factor of secondary exciter. Although the photon flux in this case is very less than x-ray tube, yet this is proven the better way to measure Rayleigh scattering cross sections.

Garg et al.[8] measured Rayleigh and Compton scattering cross sections of photons of energy 34.6 keV for 10 elements including lead (Pb) elements and some alloys at scattering angle 45° . The required photon beam was obtained by a Ce target acting as secondary source which was excited by a tungsten anode x-ray tube. Ce K-X-rays were used as incident photons. A Si(Li) detector having a resolution 190 eV was used to detect and record the data. With this resolution it is tough to resolve the $K\alpha$ X-rays of Ce, So they measured the combined peak area of both the X-rays. Measured results are reported to be higher than calculated theoretically using form factor approach. The work was concluded by emphasizing on need of further measurements.

Ajay kumar et al. (2002) [4] measured Inelastic scattering differential cross sections for the 22.1 keV photons for about 21 elements ranging from low Z to High Z at 133° . The incident photon of energy 22.1 keV were obtained from ^{109}Cd radioisotope source in the form of a monochromatic beam and the detected radiation was recorded by high purity germanium (HPGe) detector. Measurements were successfully done in the regions far above and below 22.1 keV, but it was not possible to measure the cross sections for the elements which has their K-shell binding energies in the neighborhood of incident photon energy. The measured values were showing good agreement with the theoretical values using form factor approach.

Prem singh et al. (2006) [10] measured cross sections for Rayleigh and Compton scattering of the photons of Mo $k\alpha$ X-ray with energy 17.44keV at scattering angle, 141° for the elements up to $Z = 90$. The photon source use in these measurements was ^{241}Am radioactive source and the required photon energy was obtained by using Mo foil acting as secondary source being excited by the primary Am Source. The emitted radiation was recorded by a planar HPGe. In case of elastic scattering the measured results were found to be in agreement with in 5 to 7 %. Theoretical calculations were performed using two approaches, form factor and S-matrix approach. Theoretical calculations for compton scattering cross sections were performed using the Klein-Nishina cross sections formula including the incoherent scattering function. Heavy deviation is noticed for the elements with K-shell binding energy lying in the neighbourhood of incident photon energy, which tells need to design a suitable method to measure cross sections for those elements.

Sanjiv puri et al. (1996) [9] measured scattering cross sections for the elastic scattering at incident photon energy 59.5 keV for nineteen elements in the atomic region $13 \leq Z \leq 82$ at scattering angle 130° and compared these with the theoretically evaluated cross sections using the form factor and S-matrix formalism. The monochromatic photon beam with energy 59.54 keV was taken from ^{241}Am radioactive source and the emitted photons were collected and recorded by Si(Li) detector. Here, different trends were noticed for the elements above and below the incident photon energy. The elements having K-shell binding energy less than 59.54 keV were showing values in good agreement with the theoretically evaluated values using form factor formalism. On the other hand, the elements having their K shell binding energy greater than 59.54 keV were showing their measured value in good agreement with the theoretically calculated cross section values using state of the art S-matrix approach. It is important to mention here that in case of the Dy the experimentally obtained value is lower by approx. 20% than theoretical calculated cross section values. The reason for this deviation is still not clear. The reason may be lying in its threshold value lying in the vicinity to the incident photon energy.

J.S. Shahi et al. (1997) [7] measured cross sections of the Elastic scattering for the incident photon energy 22.1 keV for 30 elements in the atomic range $12 \leq Z \leq 92$ at scattering angle 117° . The monochromatic incident photon beam of energy 22.1 keV was taken from ^{109}Cd radioisotope source. The emitted radiation was detected and recorded by Si (Li) detector. The measured values were showing good agreement with the theoretically calculated values using both of the form factor formalism and S-matrix approach.

J.S Shahi et al. (1998) [10] measured scattering cross sections for the elastic scattering of 59.5 keV photons by 42 elements in the atomic region $12 \leq Z \leq 92$ at scattering angle 121° and compared these with the theoretically evaluated cross sections using the form factor and S-matrix formalism. In this arrangement, ^{241}Am radioisotope as the photon source and a Si (Li) detector was used. The elements having K-shell binding energy less than 59.54 keV were showing values in good agreement with the theoretically evaluated values using form factor formalism. On the other hand, the elements having their K shell binding energy greater than 59.54 keV were showing their measured value in good agreement with the theoretically calculated cross section values using state of the art S-matrix approach. It is important to mention here that in case of the Erbium the experimentally obtained value is lower by approx. 12% than theoretical calculated cross section values. The reason for this deviation is still not clear. The reason may be lying in its threshold value lying in the vicinity to the incident photon energy with the difference of 2.1 keV lower side.

Gurjot singh et al. (2017) [12] measured Rayleigh scattering cross sections for three incident photon energies 45.2 keV, 46.0 keV and 52.1 keV (K X-rays of Dy) for 44 elements in range $22 \leq Z \leq 90$, at scattering angle 139° . The incident X-ray photons were produced by exciting a Dysprosium foil using ^{241}Am radioactive source. The emitted photons were detected and recorded by LEGe detector, which was successful in resolving the $K\alpha$ and $K\beta$ x-rays of Dysprosium. The measured elastic scattering cross sections were found to be in good agreement with the theoretically calculated values using the two approaches, Form factor formalism and S- Matrix approach. Again here, it was a challenge to calculate the cross sections for the elements lying near the ionization threshold.

4. Theoretical Evaluation of Rayleigh Scattering cross sections

Rayleigh scattering cross sections are calculated for the elements in range $1 \leq Z \leq 92$ at incident photon energies in the range $36.03 \text{ keV} \leq E \leq 46.00 \text{ keV}$. For calculating the Rayleigh scattering cross section values, two approaches are employed, viz., form factor formalism and state of the art S-Matrix approach.

The cross section values are calculated for incident photons of 36.03 keV, 42.00 keV, 45.21 keV and 46.00 keV energy at scattering angle 140° . It was planned to cross study the Rayleigh scattering cross sections available in literature. For this the data available at Rayleigh scattering database (RTAB) developed by Kissel et al. is used in literature and also in present work. The modified form factor cross sections and anomalous scattering factor corrected modified form factor cross sections were calculated using the modified form factor parameters (g) and anomalous scattering factors g' and g'' obtained from Rayleigh scattering database. In case of S-matrix approach the cross sections the precalculated cross section values are just picked up from the database at respective energies at the mentioned scattering angle.

It is to be noted that all the parameters and precalculated values are available at some of the energies in the database from keV to MeV. Here in case of present work, the values are available at 36.03 keV and 46.00 keV incident photon energies. It is easy to calculate the precise values of cross sections using required parameters for these two energies. But, in the case of the incident photon energies lying between these two values the cross sections are obtained by interpolating the parameter values. The Rayleigh scattering cross section calculated in the present work are listed in tables 2 to 5 for various incident photon energies at scattering angle 140° . Same are shown in plots Fig. 1 to 4. To understand the concept all the elements are listed with their respective K-shell binding energies.

Table1: List of elements with respective K shell Binding energies.

Z	Symbols	Names	B.E. (K)	Z	Symbols	Names	B.E. (K)	Z	Symbols	Names	B.E. (K)
1	H	Hydrogen	1.00797	20	Ca	Calcium	40.08	39	Y	Yttrium	88.9059
2	He	Helium	4.00260	21	Sc	Scandium	44.9559	40	Zr	Zirconium	91.22
3	Li	Lithium	6.941	22	Ti	Titanium	47.90	41	Nb	Niobium	92.9064
4	Be	Beryllium	9.01218	23	V	Vanadium	50.9415	42	Mo	Molybdenum	95.94
5	B	Boron	10.81	24	Cr	Chromium	51.996	43	Tc	Technetium	(98)
6	C	Carbon	12.011	25	Mn	Manganese	54.9380	44	Ru	Ruthenium	101.07
7	N	Nitrogen	14.0067	26	Fe	Iron	55.847	45	Rh	Rhodium	102.905
8	O	Oxygen	15.9994	27	Co	Cobalt	58.9332	46	Pd	Palladium	106.4
9	F	Fluorine	18.998	28	Ni	Nickel	58.70	47	Ag	Silver	107.868
10	Ne	Neon	20.179	29	Cu	Copper	63.546	48	Cd	Cadmium	112.41
11	Na	Sodium	22.989	30	Zn	Zinc	65.38	49	In	Indium	114.82

12	Mg	Magnesium	24.305	31	Ga	Gallium	69.72	50	Sn	Tin	118.69
13	Al	Aluminum	26.981	32	Ge	Germanium	72.59	51	Sb	Antimony	121.75
14	Si	Silicon	28.085	33	As	Arsenic	74.9216	52	Te	Tellurium	127.60
15	P	Phosphorus	30.973	34	Se	Selenium	78.96	53	I	Iodine	126.904
16	S	Sulfur	32.06	35	Br	Bromine	79.904	54	Xe	Xenon	131.30
17	Cl	Chlorine	35.453	36	Kr	Krypton	83.80	55	Cs	Cesium	132.9054
18	Ar	Argon	39.948	37	Rb	Rubidium	85.4678	56	Ba	Barium	137.33
19	K	Potassium	39.0983	38	Sr	Strontium	87.62	57	La	Lanthanum	138.9055
Z	Symbols	Names	B.K.(K)	Z	Symbols	Names	B.K.(K)	Z	Symbols	Names	B.K.(K)
58	Ce	Cerium	40.443	70	Yb	Ytterbium	61.332	82	Pb	Lead	88.004
59	Pr	Praseodymium	41.991	71	Lu	Lutetium	63.316	83	Bi	Bismuth	90.526
60	Nd	Neodymium	43.569	72	Hf	Hafnium	65.345	84	Po	Polonium	93.105
61	Pm	Promethium	45.184	73	Ta	Tantalum	67.416	85	At	Astatine	95.730
62	Sm	Samarium	46.834	74	W	Tungsten	69.525	86	Rn	Radon	98.404
63	Eu	Europium	48.519	75	Re	Rhenium	71.676	87	Fr	Francium	101.137
64	Gd	Gadolinium	50.239	76	Os	Osmium	73.871	88	Ra	Radium	103.922
65	Tb	Terbium	51.996	77	Ir	Iridium	76.111	89	Ac	Actinium	106.759
66	Dy	Dysprosium	53.788	78	Pt	Platinum	78.395	90	Th	Thorium	109.651
67	Ho	Holmium	55.618	79	Au	Gold	80.725	91	Pa	Protactinium	112.601
68	Er	Erbium	57.486	80	Hg	Mercury	83.102	92	U	Uranium	115.606
69	Tm	Thulium	59.390	81	Tl	Thallium	85.530	93	Np	Neptunium	118.670

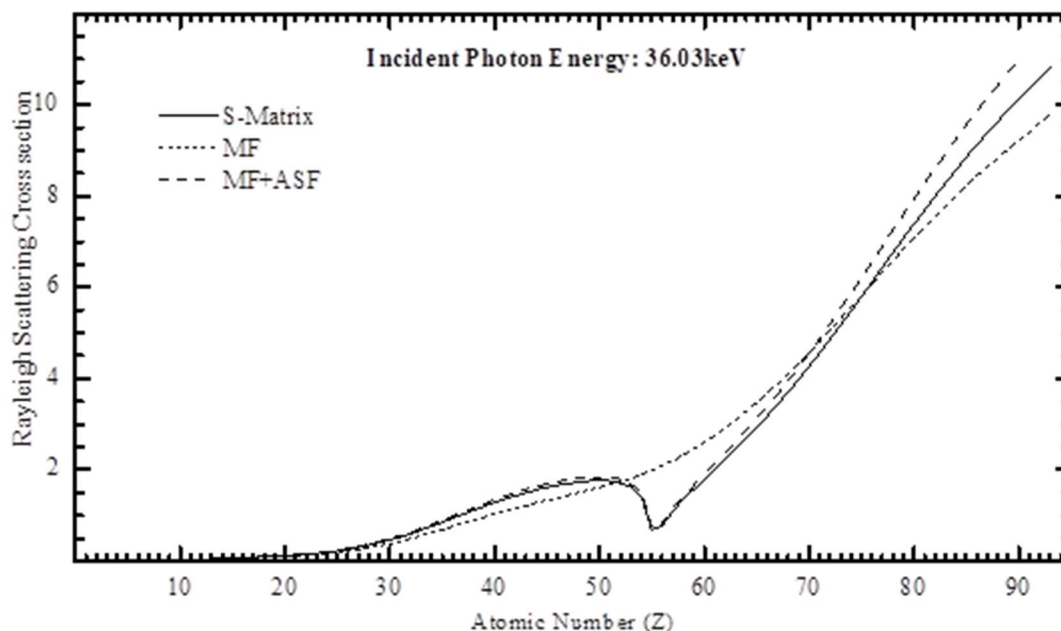


Fig. 1: Plot of theoretical Rayleigh scattering cross section values calculated at 36.03 keV.

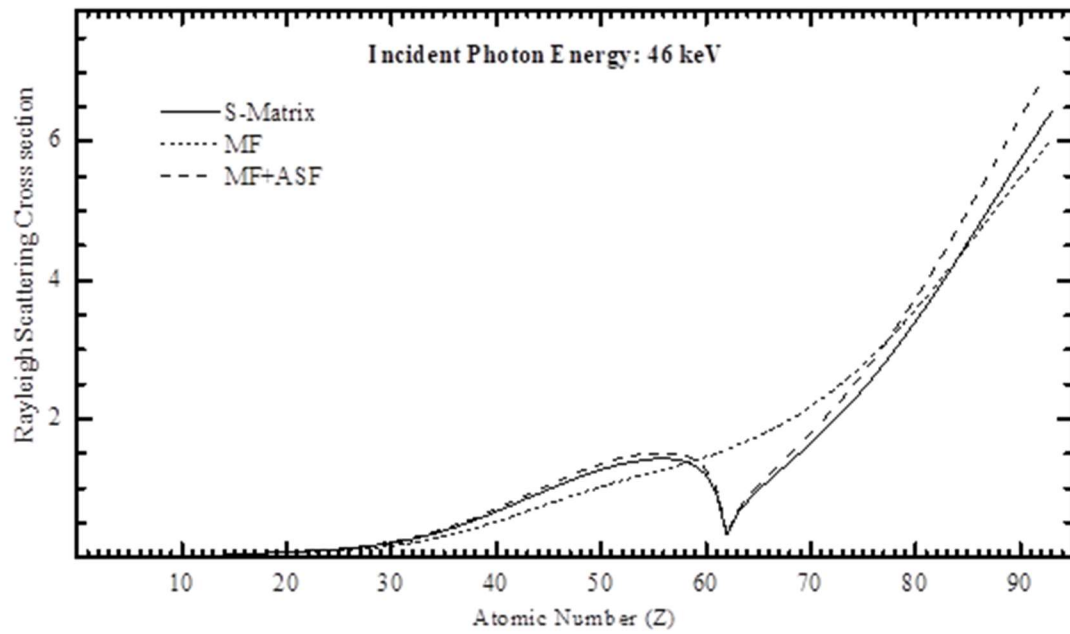


Fig. 2: Plot of theoretical Rayleigh scattering cross section values calculated at 46 keV.

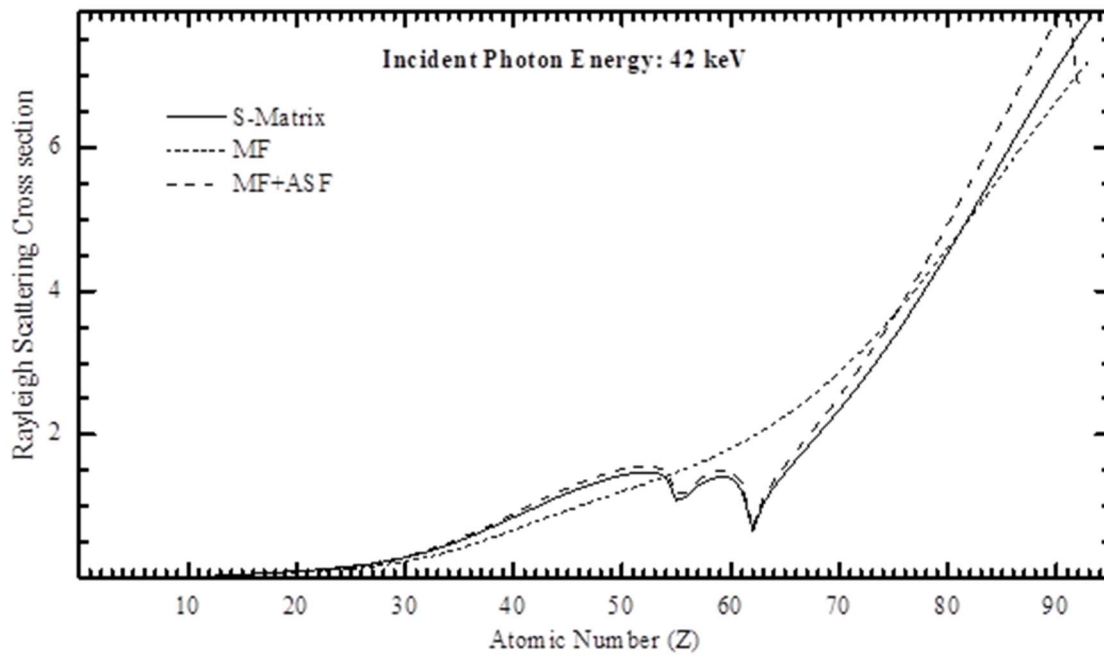


Fig. 3: Plot of interpolated theoretical Rayleigh scattering cross section values at 42 keV.

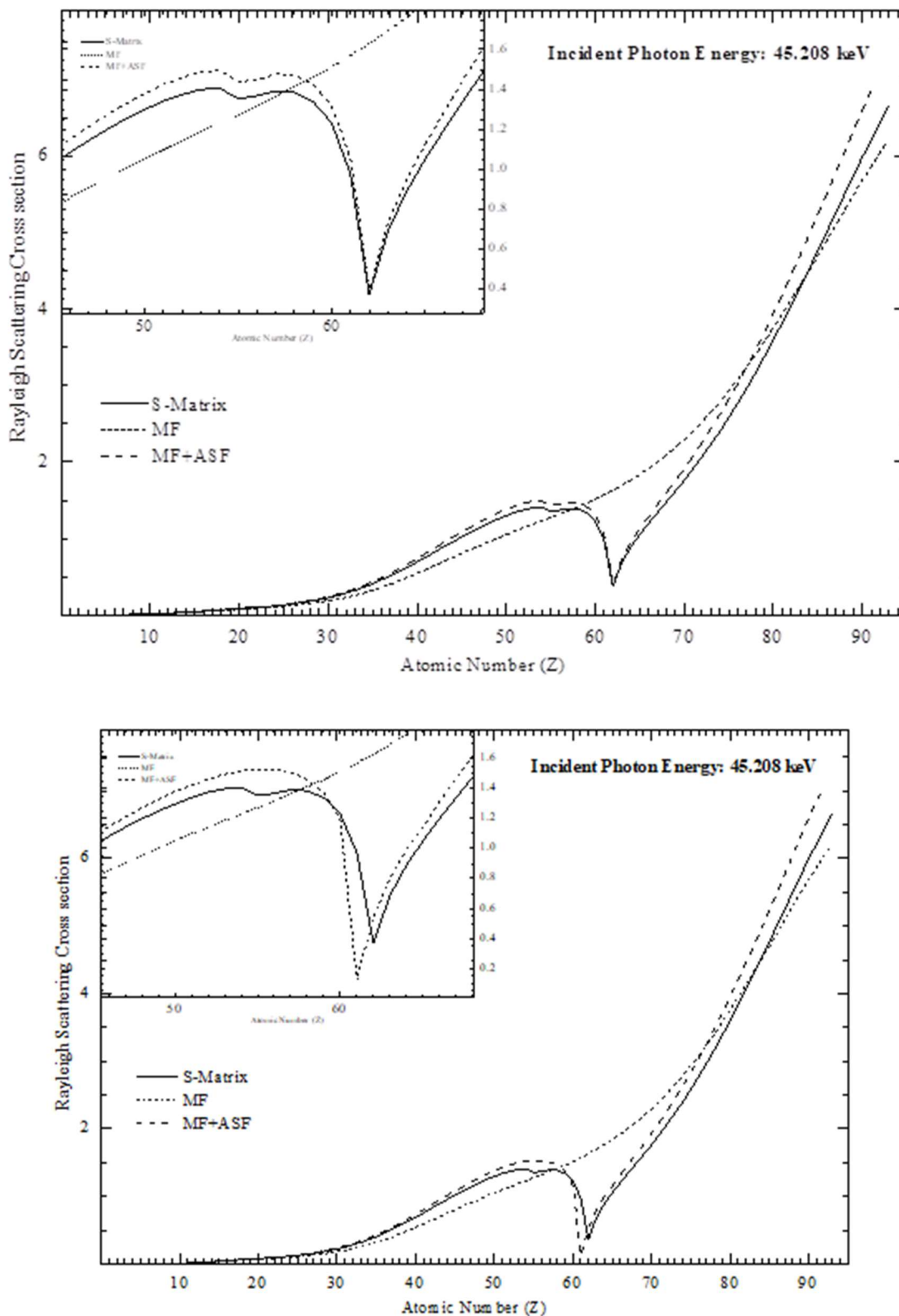


Fig. 5: Plot of corrected MFASF cross sections and values interpolated S-Matrix theoretical Rayleigh scattering cross section values

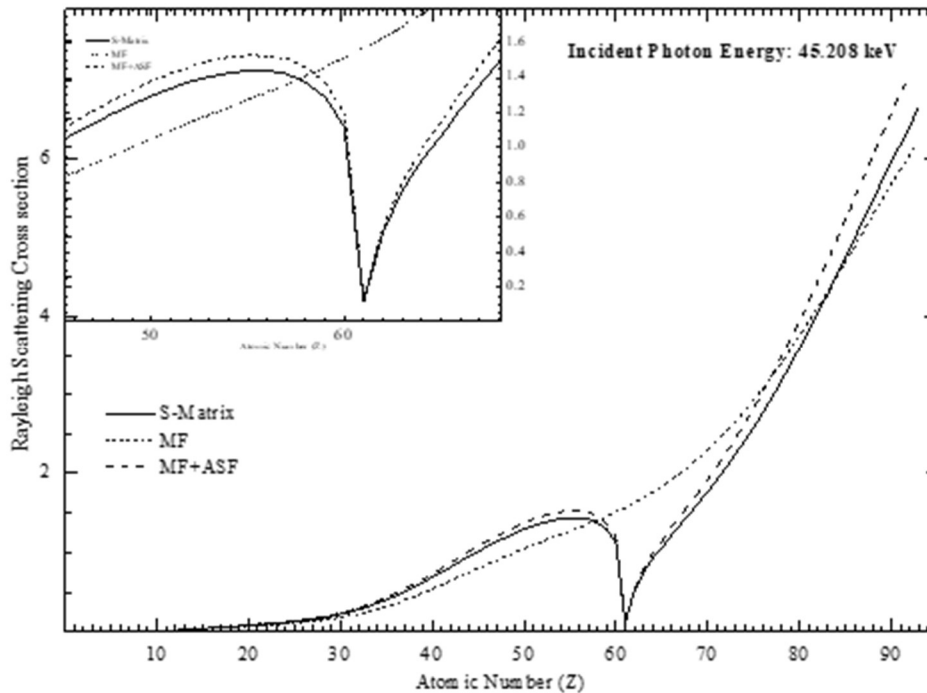


Fig. 6: Plot of S-Matrix theoretical Rayleigh scattering cross section values corrected by normalizing with corrected MFASF cross section values.

5. Results and discussions

It is clear from the plot in the Fig. 1 that values of Modified form factor cross sections keep on increasing with the atomic number. At this point the physics of the processes were contradicted by the fact that when the incident photon energy is equal to or slightly greater than the binding energy of the interacting electron, this electron leaves its position by absorbing the incident photon. The process is known as photoionization. In other words, at this value of incident photon energy the probability of the other competing processes is least as compared to photoelectron emission or photoionization. So, here at this value a reduction in the Rayleigh scattering cross section is expected. This contradiction is addressed by adding the anomalous scattering factors, which are employed as correction for the effects related to atomic structure i.e., the virtual excitation and ionization of atomic electron. Their inclusion provided the dip at the expected incident photon energy and binding energy resonance combination. The values were now known as MFASF cross section values. These theoretical cross section values are in the agreement with the values obtained using S-matrix values. Further, it is noticed that the difference between MFASF and SM cross sections keep on increasing after the dip, which is clearly visible for high Z elements.

The calculations of Rayleigh scattering cross sections becomes easy deal by using the theoretical available data. As previously mentioned that calculating the cross sections at energies given in between two energies where the values are available interpolation is involved. In present work, the problem is noticed while calculating the cross section values at 42 keV and 45.21 keV energies. Plots for both of these are shown in Fig. 3 and 4, respectively. There are two dips noticed in both cases appearing due to interpolation done to find the values in the middle of two energies. In fig. 1 at

incident photon energy 36.03 keV the dip is at $Z = 55$ and in fig. 2 at incident photon energy 46 keV the dip is at $Z = 62$. Upon careful observation one finds the positions of the dips on the same places in fig. 3 and fig. 4. Thus the method of interpolation being used by many researchers in the literature is contradicting as witnessed by present situation.

To overcome the problem, the values were manually calculated using the modified form factors (g), both of the anomalous scattering factors (g' and g'') which were again available at some fixed energies. But the difference between the alternate values of energies in ASF data is very less. So, the confidence in calculating the values is achieved using these values in scattering cross section formula. The obtained values are plotted in fig. 5 for incident photon energy 45.21 keV and it can be observed that the dip is shifted to one element to the left i.e. at $Z = 61$, which is actually the same element having K shell binding energy 45.20 keV. The only challenge is to understand how to reach the S-matrix values for which no factors are available. The researcher usually avoid comparing their experimental results in these type of cases. But Singh et al.[11] and Singh et al. used the method of normalizing the s matrix values with MFASF cross section values using the ratios between them at given energies, shown in fig. 6. where the trend and dip is very accurately matching.

6. Conclusions

It is concluded that the method of interpolations is a good tool to take the idea of the trend of the theoretical Rayleigh scattering cross section values at the incident photon energies where the values are not available in RTAB. But these should not be taken as final values as there some deviation with the actual numbers is expected. Also in case of experimental studies it is rare to observe cross section at the element present on the dip because of overlapping of K X-rays of elements on Rayleigh scatter peak, as the former has a huge count rate and later become negligible so finding the experimental value is scarce at the dip experimentally too.

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