CHAPTER - 2

THEORIES OF PHOTON - ATOM ELASTIC SCATTERING

Elastic scattering is only one of a variety of processes by which photons can interact with matter. The theory of the electromagnetic interaction, in general, between gamma quanta and the atom is called quantum electrodynamics. Quantum electrodynamic calculation methods have been successfully used for the computation of practically important processes of interaction between photons and the atoms.

2.1 Theoretical framework :

For an exact and complete description of the interaction of electromagnetic radiation with matter, both the radiation field and the atom should be treated quantum mechanically. But it is not possible to solve this problem exactly. A semi-classical treatment is therefore used in which the radiation field is treated classically and the atom is treated quantum mechanically. The atom and the radiation may be considered as composing a single system. The Hamiltonian of this system can be written down and the usual quantum mechanical treatment applied to it. The theory of the photon-atom interaction then requires finding solutions to the Schrodinger equation

$$H\Psi = i\hbar \frac{\partial \Psi}{\partial t}$$

in the vector potential of the electromagnetic field.

Even in this semi-classical framework, it is not possible to solve the problem of atom-field interaction exactly. Most of the treatments are therefore based on the perturbation theory. In it, it is assumed that the initial state of the atom is not much changed due to the interaction with radiation. The field due to the incident radiation is treated as a perturbation of the atomic field and the resulting perturbation of the atomic wave function is calculated. The determination of the perturbed wave function involves calculation of the quantities called the matrix elements of the perturbing field.

The electromagnetic interaction between the incident photon and the target atom is described by the "perturbed" Hamiltonian

$$H = \frac{1}{2m}\left(p - \frac{eA}{c}\right)^2 + U + H_\gamma$$

$$= \left(\frac{p^2}{2m} + U\right) + H_\gamma - \frac{e}{mc}\vec{p}\cdot\vec{A} + \frac{e^2}{2mc^2}A^2$$

$$= H_{atom} + H_\gamma + V_{int}$$

$$= H_o + V_{int}$$

where H_{atom} is the Hamiltonian operator of the atom, H_γ is the Hamiltonian of the radiation, A is the operator of the vector potential of the radiation field, H_o is the unperturbed Hamiltonian, and V_{int} is the interaction Hamiltonian which plays the role of perturbation. We find that

$$V_{int} = -\frac{e}{mc}\vec{p}\cdot\vec{A} + \frac{e^2}{2mc^2}A^2$$

While the first term on the right hand side corresponds to the processes of absorption (or emission), the second term leads to the processes called scattering. Atomic elastic (Rayleigh) scattering is thus fundamentally a second order quantum electrodynamic process.

2.2 Simplistic form factor approach to Rayleigh scattering :

Earliest calculations of Rayleigh scattering (the atomic elastic scattering from bound electrons) were carried out under the form factor approximation in which the binding energy of the electrons in the atom is neglected. In this method, the classical theory of scattering of X-rays by electrons is used as a basis for the calculations. The following simplifying assumptions are made[6] :

1. Each electron is so loosely bound that it scatters according to the Thomson free-electron scattering formula.

2. The scattered amplitude due to a given atom is 'f' times that due to a single free electron under identical conditions. The number f is called the atomic form factor or the atomic scattering factor of the atom.

The Thomson formula for the differential cross section of unpolarized radiation through an angle Θ is

$$\frac{d\sigma^{Th}}{d\Omega} = \left(\frac{e^2}{mc^2}\right)^2 \frac{1+\cos^2\Theta}{2} = \frac{1}{2} r_0^2 (1+\cos^2\Theta) \quad \ldots (2.1)$$

where $r_0 = e^2/mc^2 = 2.82 \times 10^{-13}$ cm is the classical electrom radius. The corresponding scattering amplitudes polarized parallel and perpendicular to the scattering plane respectively are

$$A_{\parallel}^{Th} = -r_0 \cos\Theta$$
$$A_{\perp}^{Th} = -r_0 \qquad \ldots (2.2)$$

The form factor description of the Rayleigh scattering[7-9] employs the formulas :

$$\frac{d\sigma^{R}}{d\Omega} = \frac{d\sigma^{Th}}{d\Omega} \left| f(q) \right|^2 \qquad \ldots (2.3)$$

$$\frac{d\sigma^R}{d\Omega} = \frac{1}{2}\left(|A_\perp^R|^2 + |A_{\parallel}^R|^2\right) \qquad \ldots (2.4)$$

$$A_\perp^R = -r_0 f(q)$$
$$A_{\parallel}^R = -r_0 f(q) \cos\theta \qquad \ldots (2.5)$$

$$\hbar q = \hbar(\vec{k}_i - \vec{k}_f)$$
$$q^2 = 4k^2 \sin^2\frac{\theta}{2}$$
$$k = |\vec{k}_i| = |\vec{k}_f| = \frac{\omega}{c}$$

where $\hbar q$ is the magnitude of the momentum transfer to the atom during scattering of a photon of momentum $\hbar\vec{k}_i$ into a photon of momentum $\hbar\vec{k}_f$. The atomic form factor is defined by the equation

$$f(q) = \int \rho(\vec{r})\, e^{i\vec{q}\cdot\vec{r}}\, d^3r \qquad \ldots (2.6)$$

where $\rho(\vec{r})$ is the electron number density in the atom at $\vec{r}$ and the integration extends over the atomic volume. It is obvious that in case of forward angle scattering ($\theta = 0$) q is zero and $f(0) = \int \rho(\vec{r})\, d^3r$ approaches the atomic number Z if the atom is neutral. Further, if the distribution of electrons within the atom is assumed to be spherically symmetric, $\rho(\vec{r})$ depends only on the magnitude r and we obtain

$$f(q) = \int_0^\infty 4\pi r^2 \rho(r) \frac{\sin(qr)}{(qr)}\, dr \qquad \ldots (2.7)$$

with $\rho(r)$ satisfying the condition

$$4\pi \int_0^\infty \rho(r)\, r^2\, dr = 1$$

From the point of view of quantum mechanics, the calculation of coherent scattering of radiation from electrons was first carried out by Wentzel[10] and by Waller[11]. The results obtained were found to be identical with form factor expressions provided $\rho(r)$ was put equal to $|\psi_n|^2$ where ψ_n is the atomic wave function in the state n. In principle $\rho(r) = |\psi_n|^2$ can be calculated for an atom of each element and can be used to calculate the form factor. Practically, however, Schrodinger equation is not exactly solvable for many electron atoms and approximate methods have to be adopted to determine ψ_n. The starting point of all approximate calculations on many electron atoms is the 'central field approximation'. The basic idea is that each of the atomic electrons moves in an effectively spherically symmetric potential V(r) created by the nucleus and all the other electrons. The problem is then to determine V(r). This problem is analysed by using two approaches. For complex atoms V(r) can be determined by the statistical method of Thomas - Fermi (TF)[12-13] which is valid for heavy atoms; or for any atom, and more accurately, by the self consistent Hartree[14] theory. Further improvement is obtained when exchange is included by the use of Thomas-Fermi-Dirac (TFD)[15] or Hartree-Fock-Slater (HFS)[16-18] theory. Considerable effort has been devoted for

obtaining the best atomic form factors, the emphasis being given to the use of appropriate wave functions.

While a non-relativistic derivation of the form factor method is often given, the amplitude and cross section formulas may also be derived within a relativistic framework. This is not unlikely since the basic approximation is a high energy approximation. In the latter case the charge density $\rho(r)$ corresponds to one contributed by the relativistic bound state wave functions. Two excellent tabulations of the form factors calculated for the elements of the entire periodic table and for a wide range of momentum transfer are readily available. These are :

1. The non-relativistic Hartree-Fock calculations of Cromer and Mann compiled by Hubbell et al[1]
2. The relativistic Hartree-Fock calculations by Doyle, Turner, Cromer, Weber and øverbø compiled by Hubbell and øverbø[2].

The derivation of the basic formula

$$\frac{d\sigma^R}{d\Omega} = \frac{d\sigma^{Th}}{d\Omega} |f|^2$$

of the form factor formalism neglects the binding energies of electrons in atoms and treats them as classical Thomson electrons.

Franz[7-8], in his description of the relativistic form factor, had suggested the use of a modified form factor by writing

$$\frac{d\sigma^R}{d\Omega} = \frac{d\sigma^{Th}}{d\Omega} |g|^2$$

$$g = \int \psi^* \psi \frac{mc^2}{E - V(r)} e^{i\vec{q}\cdot\vec{r}} d^3r \quad \ldots (2.8)$$

where E is the relativistic total energy of the bound electron and V(r) is the central potential at the position r.

While the f form factor results are expected to be accurate at high photon energies, an error of the order of $Z\alpha^2$ actually remains at all energies, α being the fine structure constant (= 1/137). The g form factor approach tends to correct this $O(Z\alpha^2)$ error. A tabulation of the modified relativistic form factors (MRFF) has been given by Schaupp et al[3].

2.3 Second order S-matrix element perturbative approach :

The 'exact' calculations of Rayleigh scattering should require the use of bound electron propagator if electron binding effects are to be accurately accounted for. Considerable theoretical effort has gone into developing a method of such a calculation since the mid 1950's. The second order perturbation method for the calculation of Rayleigh scattering was developed by

Brown and co-workers[19-22]. This earlier treatment employed the Fury bound interaction representation to evaluate the second order S-matrix element and made use of the Dirac Coulomb wave functions to describe the atomic electrons. The method was applied to calculate the scattering of gamma rays of energy 0.32, 0.64, 1.28 and 2.56 mc^2 by the K-shell electrons of mercury. These calculations demonstrated the applicability of the theory. Owing to the enormous computing efforts involved, calculations were restricted to the evaluation of K-shell only. Cornille and Chapdelaine[23] later extended the evaluation to 5.12 mc^2 energy.

In the next stage of development, Johnson and co-workers[24-26] improved the Brown et al's formalism with the aid of certain modifications. Instead of Coulomb wave functions, more realistic Dirac-Hartree-Fock-Slater (DHFS) wave functions were used and L- and M- shell amplitudes were calculated together with the K-shell amplitudes. Liu, Cheng and Johnson[26] also included higher order electron-electron correlation contributions arising from the fourth order S-matrix which had been neglected in the previous work. Johnson and Cheng[24] used these improvements to calculate the Rayleigh amplitudes for photon energies 100-900 keV by relatively heavy elements in the range of Z = 30 - 82. Overall discrepancies between theory and experiment were now of the order of 10%.

Major advances have occurred in recent years with the advent of modern fast computers. Computational developments have significantly improved the theoretical description of photon interaction with atom. In a comprehensive theoretical study of the Rayleigh scattering, Pratt and co-workers[27] improved upon the previous investigations in a number of ways. They have performed calculations for the scattering of photons of energies 100 eV - 10 MeV by K-, L-, M- and N-shells of atoms of various elements upto Uranium.

Kissel and Pratt developed a relativistic second order S-matrix code for the calculation Rayleigh scattering in independent particle approximation. DHFS type self-consistent potentials are used. The atom is represented by non-interacting electrons bound in a screened central potential V(r) resulting from the charge distribution of the nucleus and the atomic electrons. Starting with the second order S-matrix element of the quantum electrodynamic interaction of the bound electron with radiation, the photon wave function is expanded in a multipole series. Electron states and propagators are not expanded in V(r) but the radial wave functions of a partial series expansion are calculated numerically. For the total atom, while numerical methods are used to obtain the inner-shell amplitudes, the outer-shell amplitudes are estimated by the use of g form factors according to the following prescription[4] :

$$\mathrm{Re}\, A_{\perp}^{i} = -r_0\, g_i(q) \qquad \mathrm{Re}\, A_{\parallel}^{i} = -r_0\, g_i(q)\cos\theta$$

$$\mathrm{Im}\, A_{\perp}^{i} = \left(\frac{\sigma_i^{PE}}{\sigma_j^{PE}}\right) \mathrm{Im}\, A_{\perp}^{j} \qquad \mathrm{Im}\, A_{\parallel}^{i} = \left(\frac{\sigma_i^{PE}}{\sigma_j^{PE}}\right) \mathrm{Im}\, A_{\parallel}^{j}$$

where A^j is the contribution of the inner shells (usually k- and L-shell) obtained by numerical partial wave S-matrix calculations, σ_i^{PE} is the photoelectric cross sections for the i-th shell. Cross sections calculated according to the above programme are claimed to have an uncertainty of the order of 1% or less.

2.4 Intercomparison of theories :

In the photon energy range within which Rayleigh scattering dominates other elastic processes state-of-the-art S-matrix based calculations of Rayleigh amplitudes are purported to be the best available so far. It should be interesting to try a comparison of various form factor calculations of Rayleigh scattering with the numerical partial wave calculations of Kissel-Pratt-Roy (KPR). In fact several such comparisons have been made by a number of authors.

Pratt and co-workers[4] find that for small momentum transfers $x \leq 10\ \text{Å}^{-1}$ where x is given by

$$x = \frac{E\,(keV)}{12.4} \sin\frac{\theta}{2} \qquad \ldots (2.9)$$

the NRFF and MRFF results agree closely with KPR calculations, whereas the RFF results are too large. For larger values of x, NRFF and RFF models differ greatly from the MRFF. Similar findings suggesting the superiority of the MRFF theory have been reported in literature by Eichler et al[28], Bradley and Ghose[29], Sidappa et al[30] and Smend et al[31] who tried to discriminate between various theoretical data sets by way of comparison with experimentally measured cross sections.

A comparative study of the various sets of theoretical cross sections for a number of elements in the photon energy range 245-1408 keV has been made by Teansomprasong and Whittingham[32]. They observe that the discrepancy between RFF and KPR cross sections increases with momentum transfer (x), atomic number(Z) and the photon energy(E)with RFF results becoming far too large. The NRFF cross sections are generally quite good upto $x \simeq 10A^{o-1}$ but then increases rapidly with x, Z and E. The MRFF cross sections, on the other hand, agree closely with KPR values upto $x \simeq 40\ A^{o-1}$.

We have calculated the theoretical Rayleigh scattering cross sections for the ^{241}Am gamma rays of energy 59.54 keV from

Table 1 - Various predictions for the unpolarized photon-atom elastic scattering cross section of 59.54 keV photons

^{42}Mo

Θ (deg)	q (mc)	$d\sigma/d\Omega$ (b/atom Sr)			
		KPR	NRFF	RFF	MRFF
0	0	141.00	140.075	140.06	138.744
5	.01	85.00	86.963	87.16	85.729
10	.02	45.00	46.969	47.40	44.376
30	.06	7.16	6.604	7.56	7.300
60	.116	1.32	1.20	1.26	1.18
90	.164	0.499	0.421	0.452	0.417
120	.201	0.340	0.303	0.291	0.262
150	.225	0.335	0.284	0.282	0.250

Table 2 .

^{48}Cd

Θ (deg)	q (mc)	$d\sigma/d\Omega$ (b/atom/Sr)			
		KPR	NRFF	RFF	MRFF
0	0	184.00	182.955	182.94	180.827
5	.01	117.00	119.643	119.88	117.682
10	.02	60.90	62.829	63.38	62.152
30	.06	11.60	10.829	12.20	11.706
60	.116	1.70	1.55	1.61	1.49
90	.164	0.748	0.622	0.679	0.619
120	.201	0.573	0.522	0.470	0.422
150	.225	0.575	0.504	0.490	0.433

Table 3. ^{50}Sn

Θ (deg)	q (mc)	$d\sigma/d\Omega$ (b/atom/Sr)			
		KPR	NRFF	RFF	MRFF
0	0	199.00	198.52	198.50	196.07
5	.01	126.00	127.92	128.48	126.44
10	.02	67.30	69.89	70.39	68.89
30	.06	13.10	12.30	13.72	13.16
60	.116	1.86	1.70	1.76	1.63
90	.164	0.824	0.690	0.751	0.682
120	.201	0.660	0.532	0.571	0.510
150	.225	0.674	0.521	0.572	0.500

Table 4. ^{68}Er

Θ (deg)	q (mc)	$d\sigma/d\Omega$ (b/atom/Sr)			
		KPR	NRFF	RFF	MRFF
0	0	342.40	367.18	367.15	360.41
5	.01	231.10	257.79	258.92	251.81
10	.02	129.20	150.84	151.92	146.84
30	.06	19.20	22.78	25.67	24.30
60	.116	3.49	4.11	5.14	4.65
90	.164	0.998	1.24	1.66	1.44
120	.201	0.835	1.24	1.21	1.02
150	.225	0.983	1.32	1.44	1.20

Table 5. ^{70}Yb

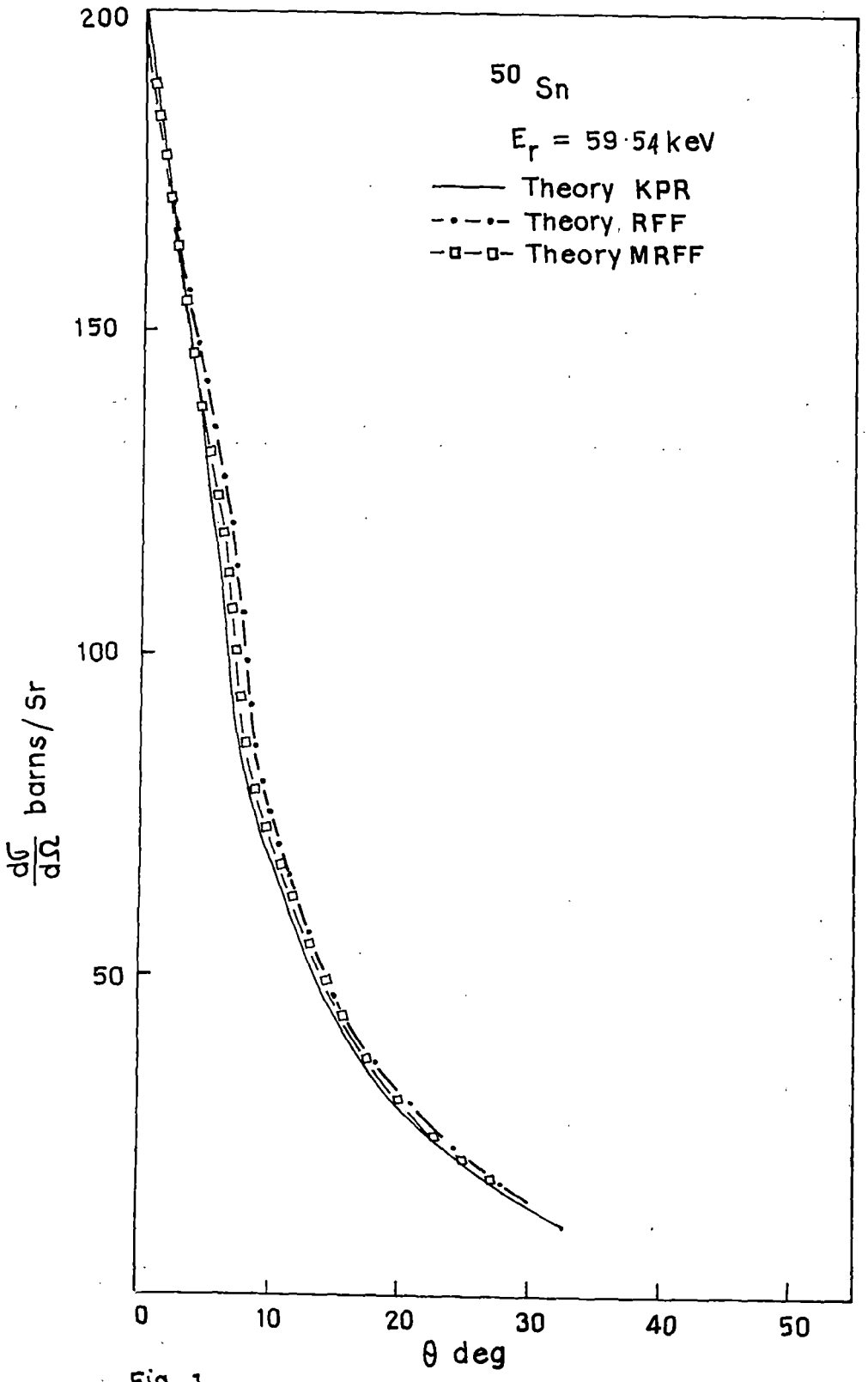
Θ(deg)	q (mc)	dσ/dΩ (b/atom/Sr)			
		KPR	NRFF	RFF	MRFF
0	0	355.30	389.10	389.06	381.69
5	.01	242.70	267.60	278.82	270.91
10	.02	136.40	157.58	165.69	159.93
30	.06	18.30	23.45	27.40	25.88
60	.116	2.88	4.32	5.65	5.10
90	.164	0.516	1.28	1.66	1.58
120	.201	0.266	1.29	1.30	1.09
150	.225	0.237	1.41	1.54	1.27

Table 6. ^{73}Ta

Θ(deg)	q (mc)	dσ/dΩ (b/atom/Sr)			
		KPR	NRFF	RFF	MRFF
0	0	400.00	423.16	423.12	414.51
5	.01	275.00	299.11	300.88	292.91
10	.02	161.00	181.57	183.79	117.65
30	.06	23.50	26.77	30.63	28.83
60	.116	4.30	5.82	6.47	5.82
90	.164	1.03	1.76	2.00	1.71
120	.201	0.630	1.41	1.49	1.24
150	.225	0.630	1.51	1.68	1.38

Table 7. ^{82}Pb

Θ (deg)	q (mc)	$d\sigma/d\Omega$ (b/atom/Sr)			
		KPR	NRFF	RFF	MRFF
0	0	423.16	423.12	414.51	400.00
5	.01	299.11	300.88	292.91	275.00
10	.02	181.57	183.79	117.65	161.00
30	.06	26.77	30.63	28.83	23.50
60	.116	7.78	8.72	7.72	6.85
90	.164	2.64	3.14	2.60	2.27
120	.201	2.03	2.18	1.76	1.44
150	.225	2.05	2.30	1.82	1.40


200
150
100
50
^{50}Sn
E_r = 59·54 keV
Theory KPR
Theory RFF
Theory MRFF
$\frac{d\sigma}{d\Omega}$ barns/Sr
0
10
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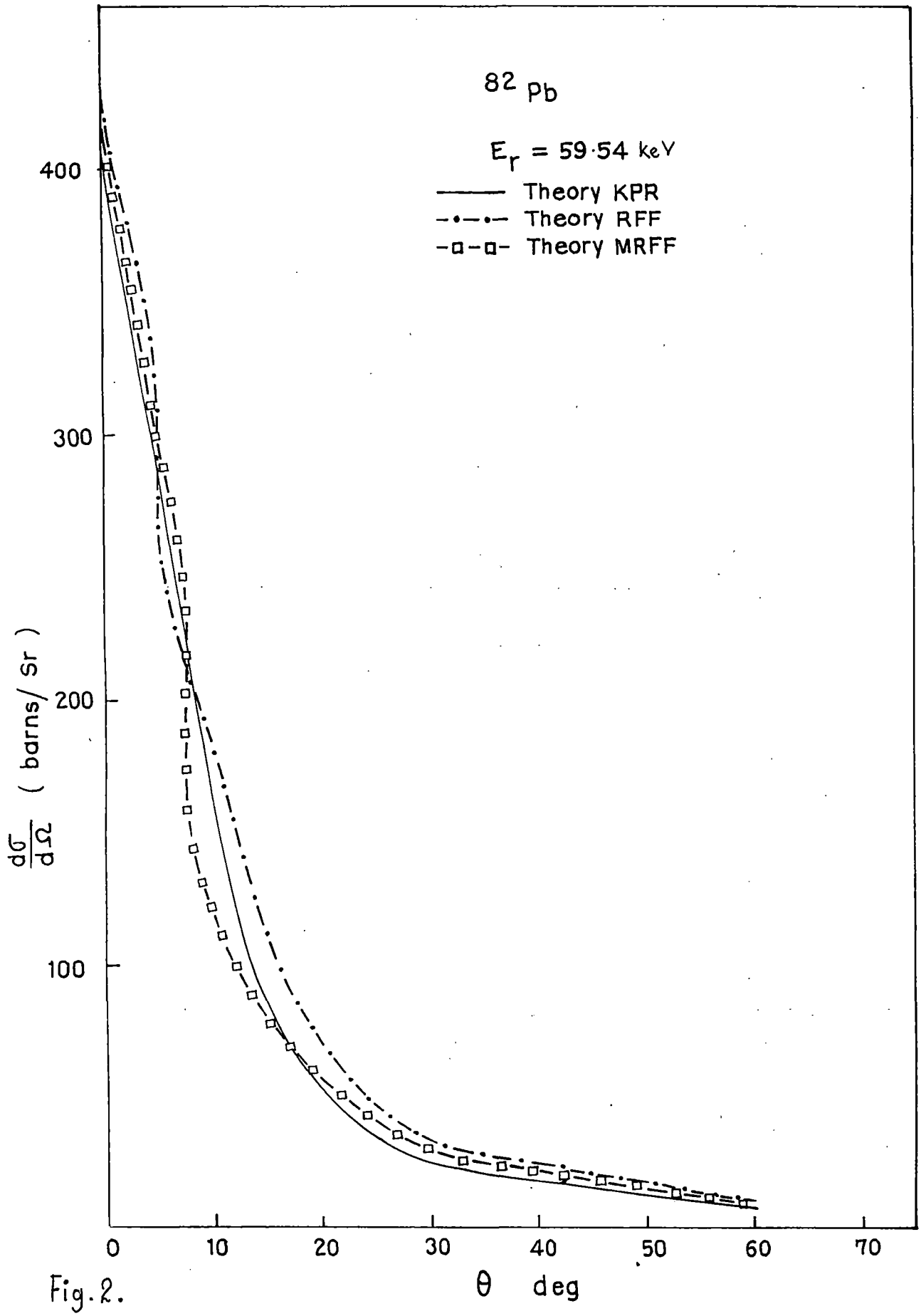
θ deg

Fig. 1.


82 Pb
E_r = 59·54 keV
Theory KPR
Theory RFF
Theory MRFF
400
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dσ/dΩ (barns/ Sr)
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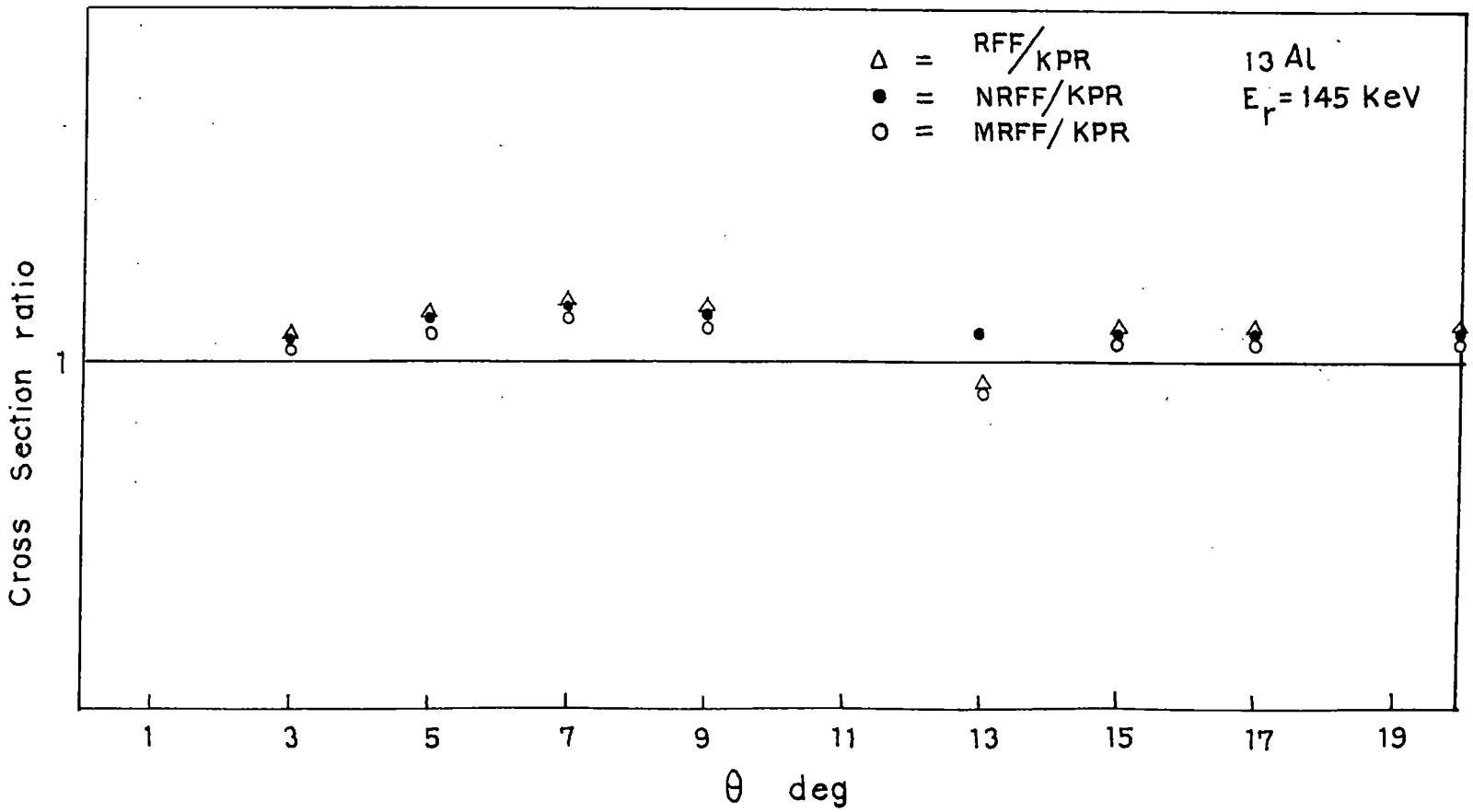
Fig. 2.


Δ = RFF/KPR
● = NRFF/KPR
o = MRFF/KPR
13 Al
E_r = 145 KeV
Cross Section ratio
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1
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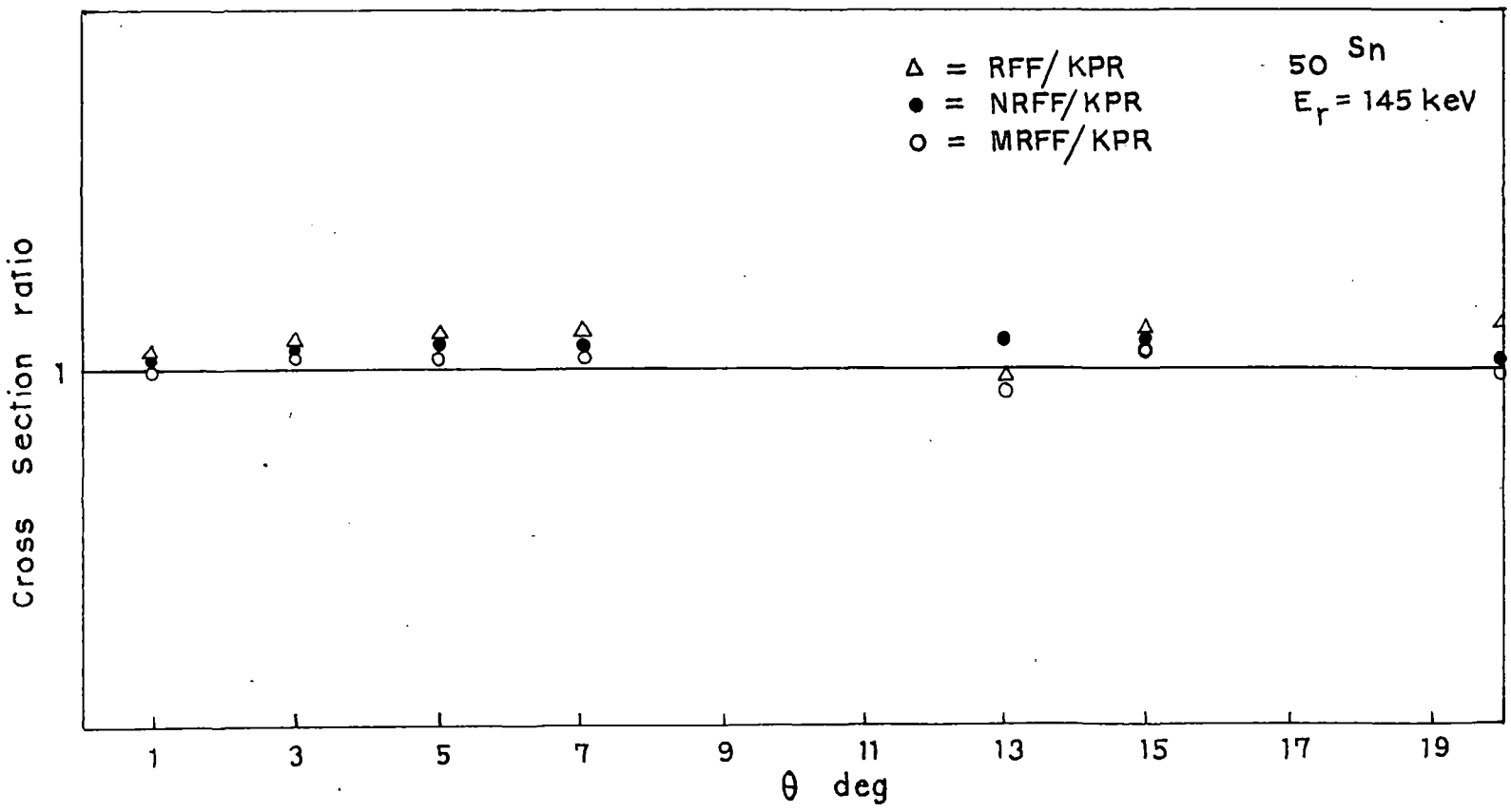
θ deg

Fig 3.


Δ = RFF/KPR
● = NRFF/KPR
o = MRFF/KPR
50 Sn
E_r = 145 keV
Cross Section ratio
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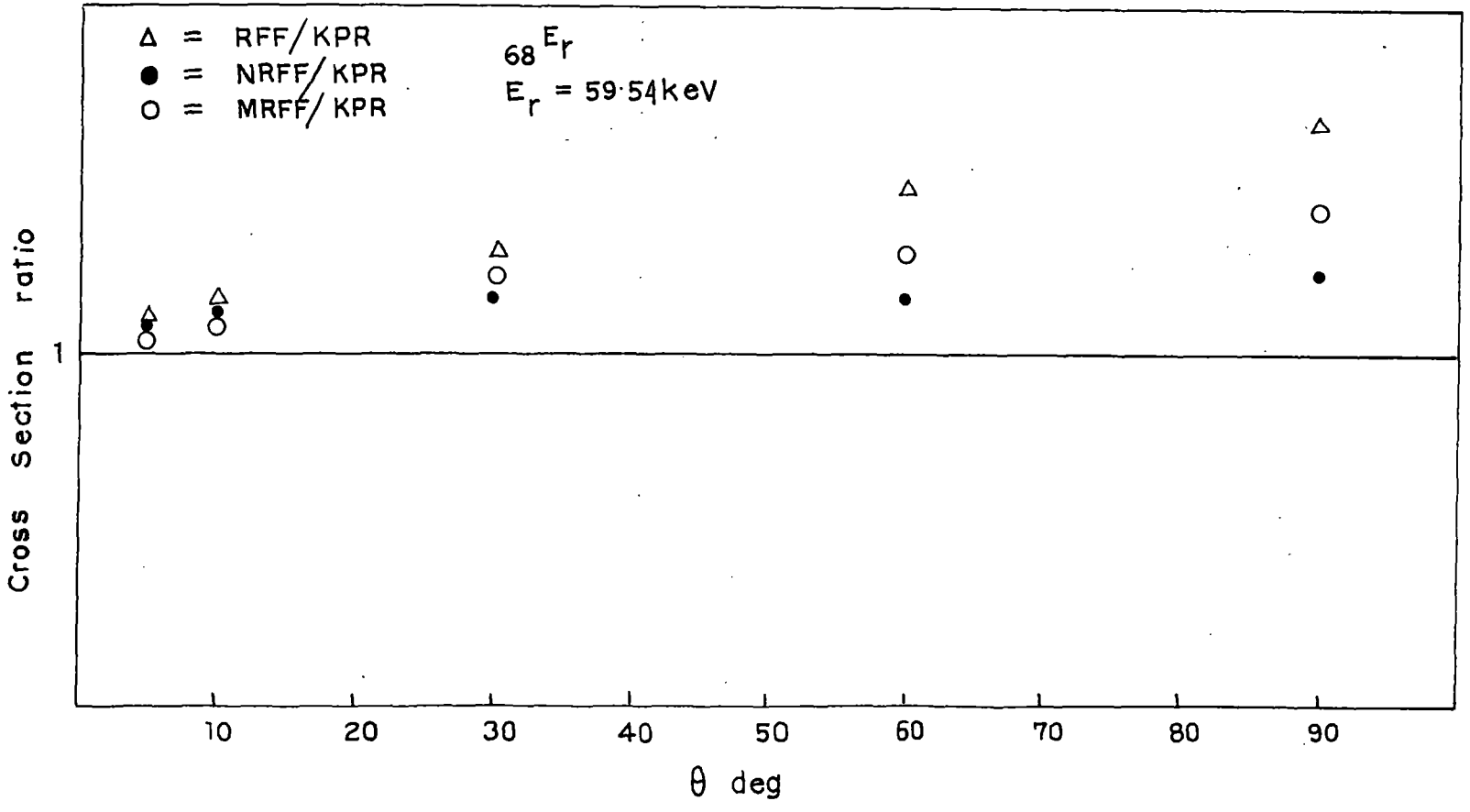
θ deg

Fig 4.


Δ = RFF/KPR
● = NRFF/KPR
○ = MRFF/KPR
68 Er
Er = 59·54keV
Cross Section ratio
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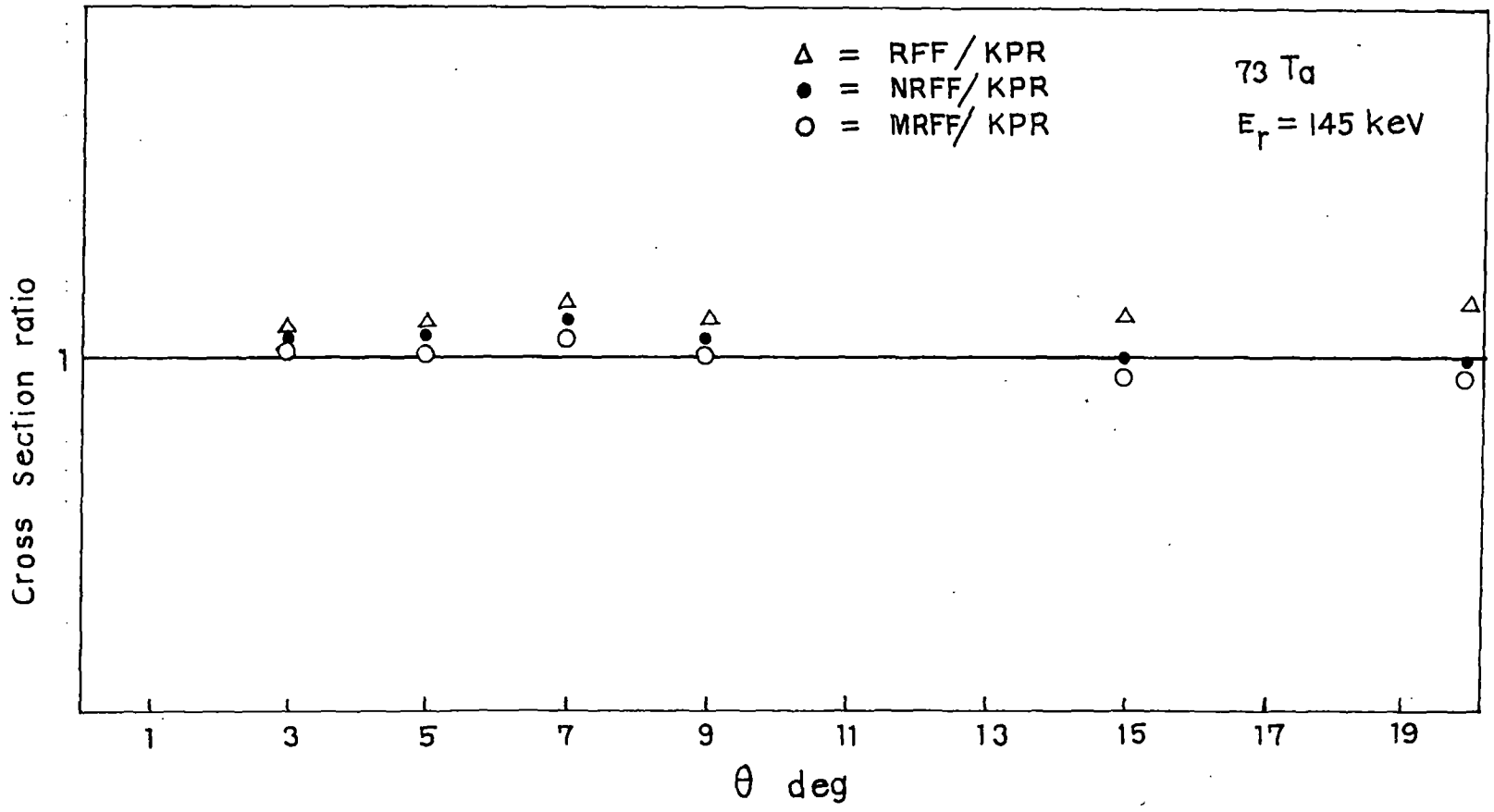
80
90
θ deg

Fig 5.


Δ = RFF / KPR
● = NRFF/ KPR
○ = MRFF/ KPR
73 Ta
E_r = 145 keV
Cross Section ratio
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θ deg

Fig 6.

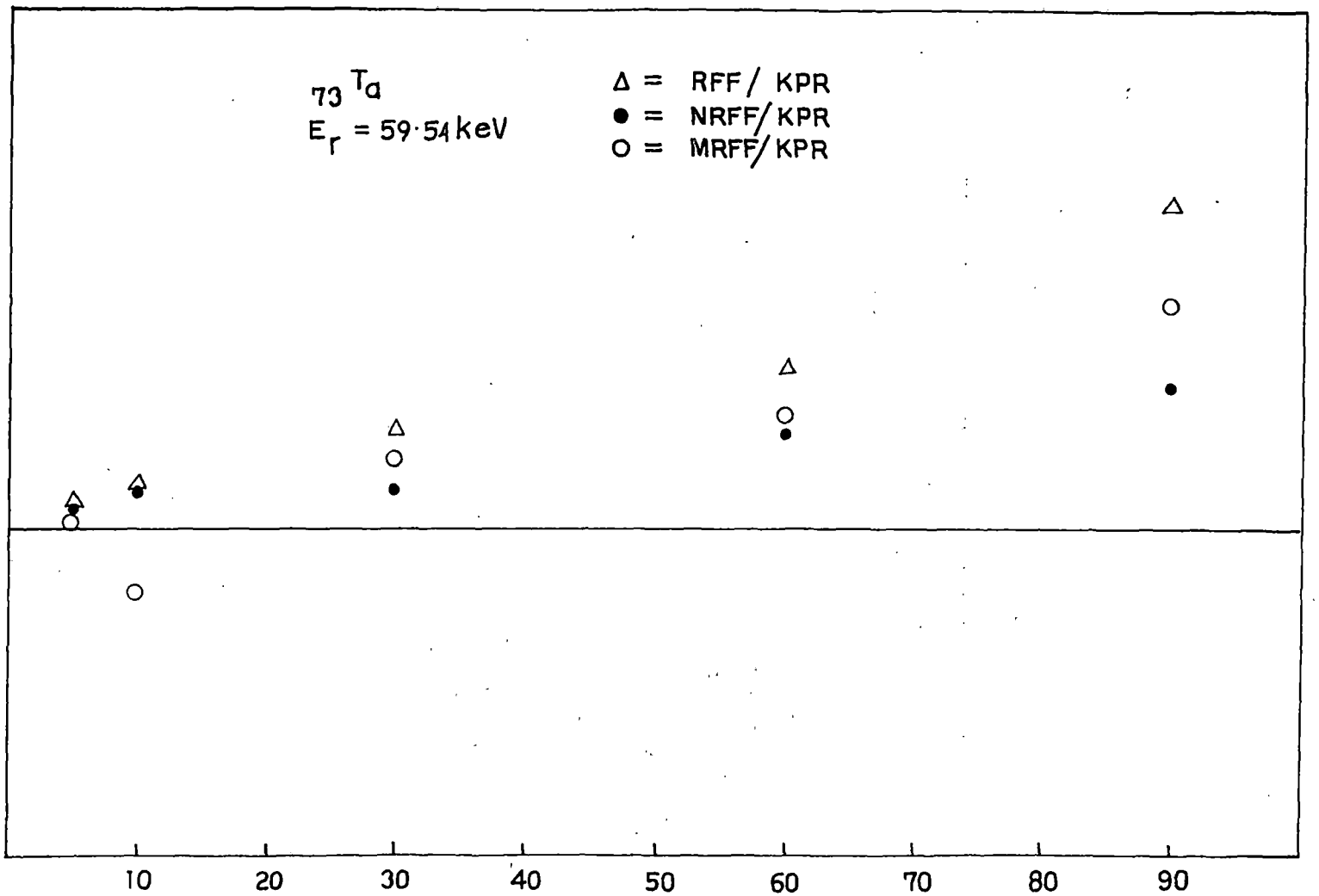
$_{73}Ta$
$E_r = 59{\cdot}54\,keV$
Δ = RFF / KPR
● = NRFF/KPR
○ = MRFF/KPR
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Fig 7.

target elements with Z = 42, 48, 50, 68, 70, 73 and 82. The NRFF, RFF and MRFF calculations were performed using the tables of Hubbell et al,[1] Hubbell and Øverbø[2] and Schaupp et al[3] respectively. The $\frac{d\sigma^{NRFF}}{d\Omega}$, $\frac{d\sigma^{RFF}}{d\Omega}$ and $\frac{d\sigma^{MRFF}}{d\Omega}$ values obtained from the calculations are given in the accompanying tables 1-7. Also given are the cross sections $\frac{d\sigma^{KPR}}{d\Omega}$ obtained from the tables of Kane et al.[4] Comparisons of various sets of cross section are also made graphically in Figs 1-7. In each of the graphs 3-7, the cross sections obtained from the various form factor calculations are plotted as ratio to the $\frac{d\sigma^{KPR}}{d\Omega}$ value.

A study of the comparison indicates that the predictions of all the theories (NRFF, RFF, MRFF and KPR) are in close agreement, and practically indistinguishable, in case of low Z elements at small angles of scattering. At larger scattering angles, and in particular for high Z elements, the RFF results are found to be larger. Of the NRFF and MRFF formulations, the latter turns out to be more successful in predicting Rayleigh scattering cross sections in coincidence with the predictions of KPR based on S-matrix formalism.