STUDY OF ELASTIC SCATTERING CROSS SECTIONS AT DIFFERENT ANGLES

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ABSTRACT

In this present study, angular dependence of the theoretical elastic scattering cross-sections has been measured. Differential cross-sections for the elastic scattering of the 59.54 keV photons have been evaluated at different angles for all the elements in the atomic region $1 \leq Z \leq 99$. The two basic theoretical approaches to calculate the elastic scattering amplitude and scattering cross-sections are form factor (FF) approximation and state of art S-matrix approach. The modified form factor (MF), modified form factor incorporating the anomalous scattering factor (MFASF) and S-matrix cross sections for all the elements have been interpolated from the values available assuming the same energy dependence as that for the MFASF values. It is observed that at forward angles, the elastic scattering cross-sections have higher values.

Keywords: Elastic, cross-section, X-rays, MF, MFASF, S-matrix

INTRODUCTION

A photon interacts with an atom through different processes involving interaction with atomic electron through photoelectric effect, scattering, i.e., elastic and inelastic scattering from electrons, and pair production around the nuclear field. In the photoelectric effect the energy of the incident photon should be either greater than or equal to the binding energy of an electron and it gets completely absorbed resulting in the emission of photoelectron with energy equal to the energy of incident photon minus the binding energy of the electron. In the elastic scattering process, the energy of the scatter photon remains same as that of the incident photon. In this process only the momentum is transferred, i.e., direction of the scatter photon changes [1-4]. The elastic scattering from the bound electrons, at lower photon energies, gives the dominant contribution to the photon-atom scattering amplitude, which is known as Rayleigh scattering. The scattering of photons from a virtual electron-positron pair created in the field of nucleus is called Delbruck scattering. In the inelastic process, the energy as well as momentum of the scatter photons changes. Inelastic scattering is of two types, i.e., Compton scattering and Raman scattering. Compton scattering is the inelastic scattering resulting in ionization of the atom and Raman scattering involves excitation of the interacting electron to higher energy unoccupied bound state. In case the incident photon energy is slightly less than binding energy of interacting electron, it proceeds by creation of a virtual hole in the respective shell/sub shell with the corresponding electron excited to an unoccupied state. Simultaneously, an electron from a higher-shell fills this hole followed by emission of a photon whose energy corresponds to the difference between final and initial holes. It can also result in a radiationless transition. The term resonant Raman scattering (RRS) has been usually employed whether the excited electron is in bound state or occupies a continuum state. When the energy of incident photon exceeds $2m_oc^2 > 1.02$ MeV, it interacts with the Coulomb field of a nucleus and the incident photon disappears with the creation of an electron-hole pair. This process of interaction of photon with atom is known as pair production. Basic photon-atom interaction processes in the x-ray energy region are shown in figure 1. The term cross-section is used as a measure of probability of the occurrence of a particular interaction process.

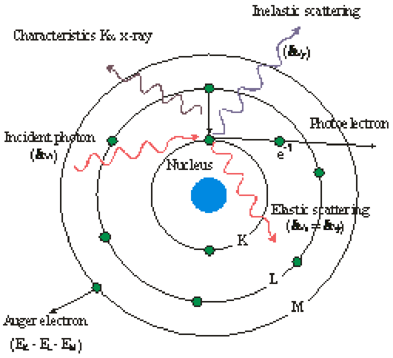

Figure 1: Basic photon-atom interaction processes in the x-ray energy region.

The inelastic scattering becomes the dominating process at ~100 keV for low-Z elements and ~500 keV in case of high-Z elements. The measurements of elastic scattering crosssections in various elements at incident photon energies close to the binding energies will be useful to explore the need of modification and the better understanding of the theory.

The elastic scattering of photons from atom involves no transfer of energy and there exist a phase relationship between the incident and scattered photons. An isolated atom itself is a composite system of nucleus and bound electrons. The scattering of photons from bound electrons is known as Rayleigh scattering. In the x-ray energy region (< 100 keV), the scattering the scattering from the nucleus is very small and Rayleigh scattering is the only domiating elastic scattering process. In case of rayleigh scattering , the scattering contribution from the bound electrons in a given atom has definte phase relationship to each other. Therefore Rayleigh scattering is also known as coherent scattering. The internal state of the atom is same after the scattering process, only some momentum has to be transfered during the scattering process. For momoatomic gases, incdent photon of energy 10 keV transfer large momentum and scattering is no more coherent. But in case of solid, the recoil momentum is transferred to the whole crystal andscattering from the different atoms in crystal will be coherent. The two basic theoretical approaches to calculate the Rayleigh scattering amplitude and scattering cross-sections are form factor (FF) approximation and state of art S-matrix approach.

FORM-FACTOR FORMALISM

The Thomson differential scattering cross section for scattering of unpolarized photons by a classical free electron is given by

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

Here σ is the scattering angle and r_o is the classical radius of the free electron.

The atomic form factor for a spherical symmetric atom containing one electron is given by

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

where τ(r) is the electron density at distance r from the centre of the atom and $\hbar q = 2(h\pi_i/c)\sin(\sigma/2)$ is the momentum transfer to the atom as the photon is scattered. The scattering cross-section in the form factor formulation is obtained from the Thomson formula as

$$\left(\frac{d\sigma}{d\Omega}\right)_{el} = \left(\frac{d\sigma}{d\Omega}\right)_T \left|f(q)\right|^2 \qquad (3)$$

The form factor approximation gives generally good predictions for the total cross-sections for photon energies above the K-shell threshold. An improved version of Form factor (FF) includes electron binding energy corrections is commonly known as the modified form factor g(q) [5]. The modified form factor for a given electron is given by

$$g(q)=4\pi\int\rho(r)\frac{\sin(qr)}{qr}\frac{mc^2}{E_i-V(r)}r^2dr \qquad (4)$$

where E_i is the total energy of the ith electron, V(r) is the atomic potential and ρ(r) is the charge distribution associated with the i^{th} electron. When non-relativistic and relativistic individual electron and total atom wavefunctions are used to derive the charge density, the resulting form factor is called non-relativistic (NF) [6] and relativistic (RF) [7] form factor, respectively. It has been found that of all form factors, modified form factor (MFF) is the best, while non-relativistic form factor (NFF) is found to be better than the relativistic form factor (RFF). In order to make the form factor valid at lower energies corrections known as the `anomalous scattering factor' have been used. Cromer and Libermann [8] computed the anomalous scattering factor (non-relativistic) f' and f'' and tabulated them for all elements Z=3-98 I the photon energy range 1 to 70 keV. Henke *et al.* [9] also tabulated the anomalous scattering factor for all elements Z=1-92 and for photon energies 0.05 to 30 keV. Corrected form factor will be then $f(q,z)=f_o(q,z)+f'+if''$. It has been revealed initially from the S-matrix values energy limits $f'(\infty)$ used by Cromer and Libermann and by Henke is not correct. The correct values have been tabulated for all neutral atoms by Kissel and Pratt [10]. At large angle of scattering, the correction term improves the scattering cross-section by about 40% and it has been demonstrated that the use of correct high energy limit removes the discrepancy between values [11].

S-MATRIX APPROACH

S-matrix approach is the best possible theoretical method to calculate the elastic scattering cross-sections. The S-matrix is an operator that connects the final scattered state of a time dependent system with an initial state. In Rayleigh scattering, the matrix element $S_{ij}=<f|S|i>$ represents the amplitude of a specific stationary state $|j\rangle$ that evolved through scattering from the initial state $|i\rangle$. In this approach, the interaction of electrons and positrons with atomic field is included in the unperturbed Hamiltonian of the Feynman-Dyson formulation of quantum electrodynamics, while the interaction with radiation filed is treated as perturbation. The Feynman diagram for the absorption first, where the incident photon of energy $h\nu_i$ is first absorbed by the initial state of the electron at time t_1 and emission first in which the final photon of energy $h\nu_i$ is emitted at time t_1 is shown in figures.2(a) and 2(b). Tabulated values of Rayleigh scattering cross sections [12] are available for the almost all the elements at seven selected photon energies of experimentalist choice in 65 angular set-ups in the energy range 0 ≤θ≤ 180°.

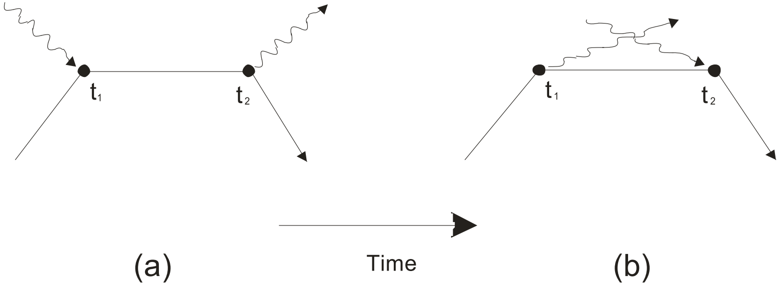

Figure 2: Feynman diagram for the Rayleigh scattering amplitude (a) absorption first (b) emission first contribution

The present study focuses on the angular dependence of the elastic scattering cross-sections in the elementscovering the atomic region 1 ≤ Z ≤ 99 for the 59.54keV photons at different angles. The results are given below. The results are better presented in figure 3 to 5.

Table 1: Elastic Scattering Cross-sections for elements with 1 ≤ Z ≤ 99 at 59.54 keV at an angle of 25°

Atomic number (Z)	SM value (milli barn/sr)	MFASF value (milli barn/sr)	MF value (milli barn/sr)
1	0.0025745	0.0025748	0.0025745
2	0.588	0.588	0.588
3	7.178	7.177	7.175
4	26	27	26
5	55	55	55
6	85	85	85
7	111	111	111
8	132	132	132
9	154	154	154
10	183	183	182
11	224	225	223
12	286	287	285
13	378	379	375
14	505	506	501
15	671	673	665
16	875	877	866
17	1111	1113	1098
18	1367	1369	1349
19	1627	1630	1604
20	1876	1880	1846
21	2098	2104	2061
22	2301	2307	2256
23	2489	2496	2435
24	2666	2674	2601
25	2839	2848	2763
26	3015	3027	2928
27	3202	3215	3101
28	3406	3421	3290
29	3633	3649	3500
30	3894	3913	3742
31	4198	4220	4026
32	4557	4581	4360
33	4981	5005	4755
34	5472	5499	5217
35	6039	6068	5749
36	6686	6716	6357
37	7404	7437	7033
38	8186	8223	7772
39	9022	9064	8563

40	9905	9952	9399
41	10833	10883	10275
42	11782	11836	11173
43	12730	12786	12068
44	13701	13767	12995
45	14648	14719	13894
46	15590	15667	14792
47	16469	16552	15632
48	17299	17389	16428
49	18087	18182	17188
50	18829	18931	17911
51	19532	19640	18602
52	20207	20321	19277
53	20864	20983	19944
54	21527	21645	20623
55	22198	22319	21327
56	22900	23024	22077
57	23623	23747	22868
58	24227	24353	23571
59	24879	25005	24349
60	25526	25656	25165
61	26162	26291	26011
62	26781	26910	26897
63	27405	27508	27826
64	28042	28149	28889
65	28422	28531	29826
66	28727	28840	30905
67	28741	28855	32041
68	28073	28185	33236
69	20143	20219	34495
70	28936	29052	35819
71	31848	31993	37318
72	34229	34393	38913
73	36462	36642	40603
74	38664	38845	42379
75	40863	41068	44248
76	43102	43329	46204
77	45377	45620	48228
78	47702	47955	50309
79	50108	50376	52501
80	52448	52731	54633
81	54810	55110	56797
82	57168	57483	58960
83	59508	59841	61114
84	61831	62179	63254
85	64195	64501	65380
86	66416	66801	67493
87	68707	69113	69611
88	71005	71414	71744

89	73330	73763	73330
90	75638	76095	76042
91	78130	78612	78386
92	80549	81043	80649
93	82947	83467	82912
94	85372	85917	85208
95	87727	88297	87442
96	90052	90627	89636
97	92370	92968	91855
98	94626	95249	94030
99	96857	97505	96183

Table 2: Elastic Scattering Cross-sections for elements with $1 \le Z \le 99$ at 59.54 keV at an angle of 45°

Atomic number (Z)	SM value (milli barn/sr)	MFASF value (milli barn/sr)	MF value (milli barn/sr)
1	0.0000275	0.0000275	0.0000275
2	0.011	0.011	0.011
3	0.247	0.247	0.247
4	1.58	1.58	1.58
5	5	5	5
6	13	13	13
7	23	23	23
8	36	36	36
9	49	49	49
10	62	62	62
11	74	75	74
12	86	86	85
13	97	98	96
14	109	110	108
15	124	125	122
16	143	144	140
17	168	169	164
18	201	203	196
19	244	246	237
20	298	302	289
21	363	368	352
22	439	444	424
23	525	532	506
24	617	625	593
25	721	730	691
26	827	838	791
27	935	948	892
28	1043	1059	992
29	1148	1165	1088
30	1256	1275	1187
31	1362	1384	1283

32	1464	1489	1375
33	1564	1590	1462
34	1660	1688	1546
35	1752	1783	1626
36	1845	1877	1704
37	1936	1971	1782
38	2030	2068	1861
39	2131	2171	1947
40	2239	2283	2040
41	2361	2407	2145
42	2496	2546	2262
43	2649	2702	2396
44	2819	2877	2549
45	3012	3074	2723
46	3228	3295	2919
47	3468	3540	3139
48	3733	3810	3385
49	4023	4105	3656
50	4336	4425	3953
51	4670	4766	4273
52	5025	5126	4617
53	5394	5502	4981
54	5778	5889	5360
55	6164	6283	5754
56	6552	6678	6157
57	6938	7066	6565
58	7263	7393	6927
59	7590	7724	7308
60	7892	8030	7685
61	8165	8304	8053
62	8402	8543	8414
63	8611	8741	8766
64	8764	8897	9120
65	8821	8956	9442
66	8780	8916	9766
67	8565	8701	10080
68	8008	8138	10386
69	4332	4409	10685
70	7584	7701	10976
71	8534	8688	11264
72	9197	9374	11549
73	9745	9942	11833
74	10245	10447	12117
75	10681	10915	12401
76	11113	11363	12691
77	11534	11799	12988
78	11956	12240	13298
79	12377	12678	13618
80	12816	13133	13962

81	13269	13603	14324
82	13743	14097	14715
83	14240	14613	15132
84	14764	15153	15577
85	15347	15728	16056
86	15904	16333	16571
87	16522	16974	17118
88	17172	17640	17701
89	17861	18355	17861
90	18573	19095	18965
91	19297	19846	19628
92	20064	20637	20331
93	20856	21459	21066
94	21672	22301	21824
95	22522	23181	22622
96	23410	24093	23455
97	24307	25019	24306
98	25227	25971	25189
99	26172	26950	26099

Table 3: Elastic Scattering Cross-sections for elements with $1 \leq Z \leq 99$ at 59.54 keV at an angle of 90°

Atomic number (Z)	SM value (milli barn/sr)	MFASF value (milli barn/sr)	MF value (milli barn/sr)
1	0.00000014	0.00000015	0.00000014
2	0.0000733	0.0000740	0.0000733
3	0.0022	0.0023	0.0022
4	0.0204	0.0206	0.0204
5	0.10	0.10	0.10
6	0.34	0.34	0.34
7	0.88	0.89	0.87
8	2	2	2
9	3	4	3
10	6	6	6
11	9	9	9
12	13	13	12
13	17	17	17
14	22	22	21
15	26	27	26
16	31	32	30
17	36	37	35
18	41	41	39
19	45	46	43
20	50	51	47
21	54	56	51
22	59	61	55
23	65	67	60
24	71	74	65

25	78	81	71
26	86	90	77
27	96	100	85
28	107	112	94
29	119	125	105
30	134	141	117
31	151	159	131
32	171	180	148
33	194	203	166
34	219	230	187
35	247	259	210
36	278	291	236
37	311	326	263
38	347	364	293
39	385	403	324
40	424	445	356
41	464	487	388
42	506	530	422
43	549	574	456
44	589	618	490
45	630	661	523
46	670	703	555
47	710	745	587
48	749	786	619
49	786	825	649
50	821	863	678
51	855	900	706
52	888	934	734
53	918	966	761
54	949	998	788
55	977	1028	814
56	1004	1057	841
57	1030	1085	869
58	1056	1112	899
59	1080	1137	931
60	1102	1160	965
61	1122	1181	1001
62	1138	1197	1040
63	1154	1210	1082
64	1159	1216	1127
65	1153	1210	1176
66	1126	1185	1229
67	1065	1122	1285
68	937	991	1346
69	404	443	1411
70	593	616	1480
71	806	846	1555
72	969	1020	1634
73	1113	1174	1719

74	1261	1320	1809
75	1382	1462	1904
76	1515	1605	2004
77	1648	1748	2108
78	1785	1895	2217
79	1923	2044	2330
80	2065	2196	2447
81	2209	2351	2566
82	2357	2509	2689
83	2505	2669	2814
84	2656	2831	2940
85	2820	2995	3067
86	2962	3158	3194
87	3114	3323	3321
88	3265	3485	3447
89	3418	3651	3418
90	3566	3813	3695
91	3706	3968	3810
92	3848	4122	3925
93	3984	4274	4037
94	4116	4420	4144
95	4246	4565	4250
96	4378	4708	4355
97	4499	4844	4453
98	4618	4979	4552
99	4735	5111	4646

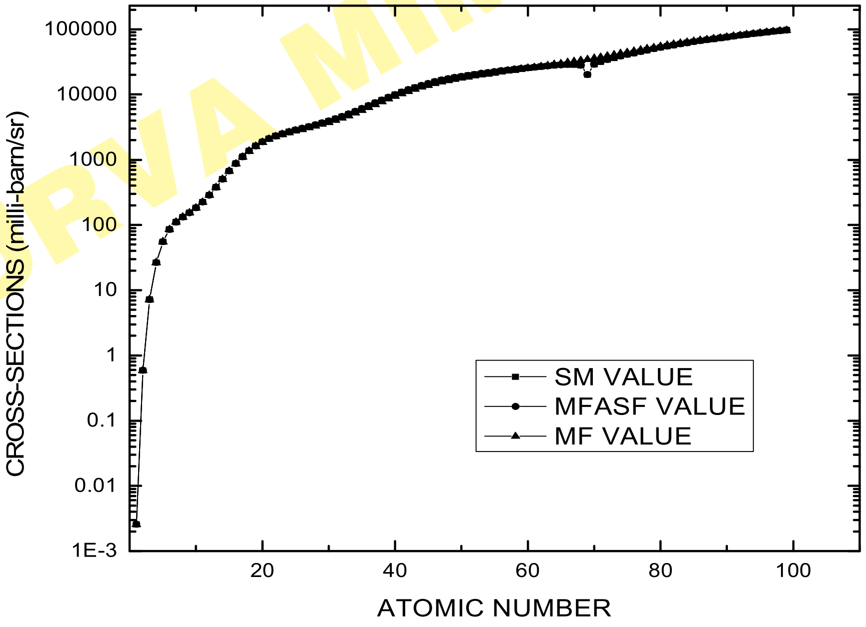

Figure 3: Elastic Scattering Cross sections for elements with 1 ≤ Z ≤ 99 at 59.54 keV at an angle of 25°

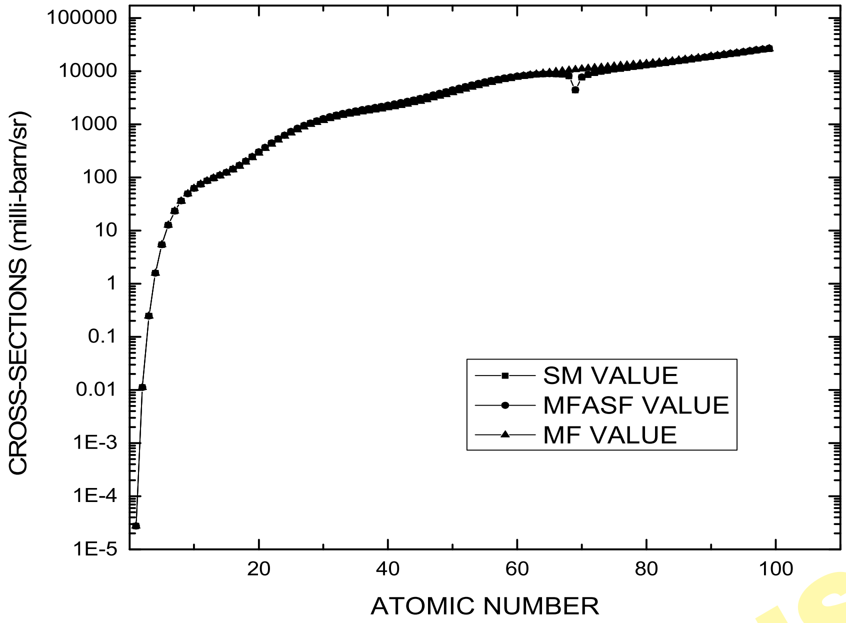

Figure 4: Elastic Scattering Cross sections for elements with 1 ≤ Z ≤ 99 at 59.54 keV at an angle of 45°

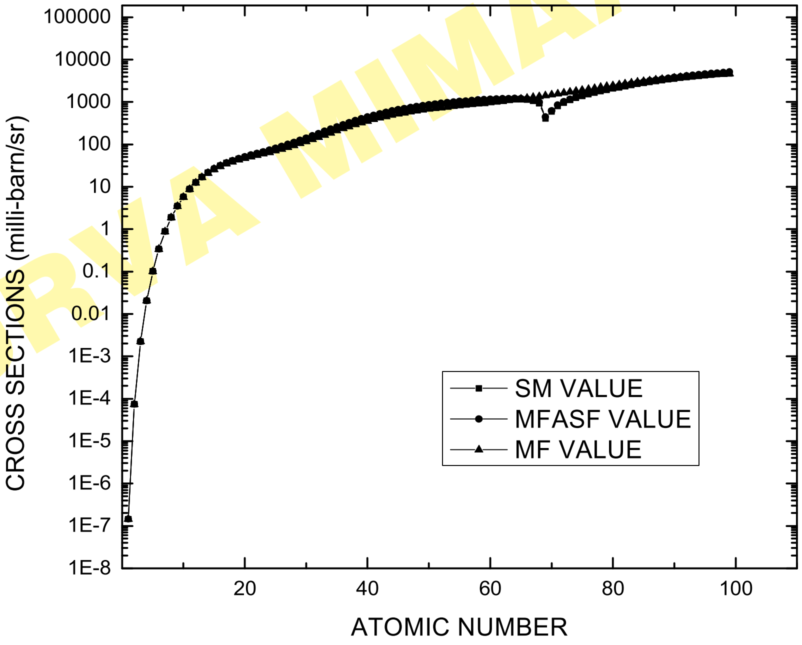

Figure 5: Elastic Scattering Cross sections for elements with 1 ≤ Z ≤ 99 at 59.54 keV at an angle of 90°

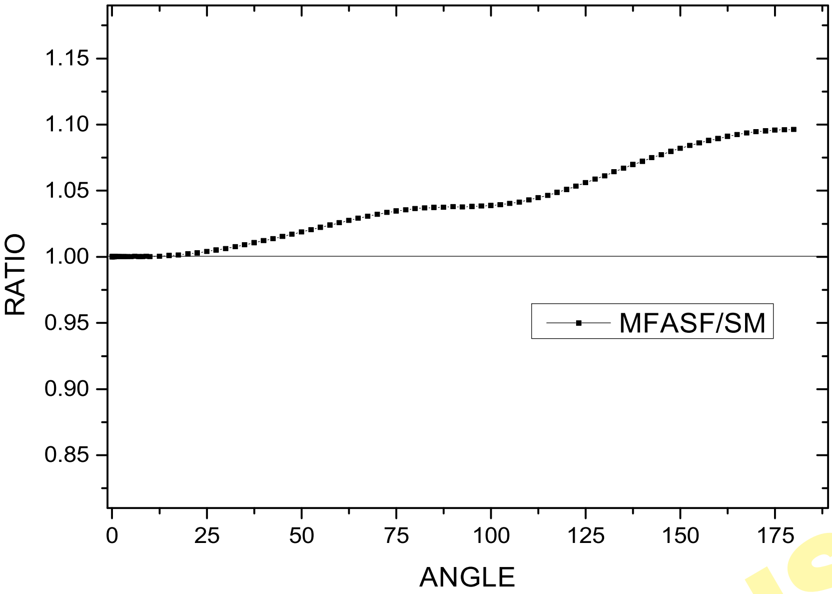

Figure 6: The ratio of MFASF to SM Scattering Cross-sections for element with atomic number 70 at 59.54 keV at different angles

The theoretical elastic scattering cross-sections in different elementsexhibit almost linear angular dependence around 140°. The average theoretical cross-section, evaluated by taking the weighted average of cross-sections at various scattering angles in proportion to the number of scattered photons agrees within 1% with the theoretical value at 140°. The MF, MFASF and S-matrix elastic scattering cross-sections are taken from Ref. [12]. Systematically computed second order S-matrix values are available for photon energies less than 300 times the K-shell binding energy on a 52 point grid of energies of experimental interest in the range 0.0543-2754.1 keV for the elements with $1 \leq Z \leq 103$. The MF, MFASF and S-matrix cross-section values for all the photon energies in all the elements under investigation have been interpolated from the values available assuming the same energy dependence as that for the MFASF values. The angular dependence of the theoretical cross-sections at forward angles as a function of scattering angle are shown in figures 3 to 5. The ratio of MFASF to SM values is shown in figure 6. The elastic scattering cross-sections at forward angles are very large.MF, MFASF and S-matrix scattering cross-sections are compared in Figures 1 to 8. These theoretical values have been taken from calculations of Kissel [12]. The ASFs, g' and g'', calculated using the relativistic Hartree-Fock-Slater potential with Latter tail have been used for theMFASF cross-sections. The ASFs have been taken to be angle independent and hence, the momentum transfer is no more a well-defined parameter for the MFASF cross-sections.The MF cross-sections at the forward angles exhibit peaked deviations, becoming few times the MFASF and SM values for the elements with binding energy equivalent to the incident energy. The MFASF and S-matrix cross-sections, in general, follow the similar trend over the whole atomic region.

CONCLUSION

In the present results, it is observed that the elastic scattering cross-sections at such low energy are significant enougheven for the low-Z elements. The scattering information available in the energy dispersive x-ray fluorescence (EDXRF) measurements is useful for analytical applications related to the low-Z elements and hydrogen in the hydrogen-rich samples.

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