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Compton profile of samarium

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Abstract : The Compton profile of Sm has been measured using IGP Type Coaxial photon detector The target atoms were excited by means of 59 54 keV gamma rays from Am-241 radioactive source of strength 300 mCi. Elemental foil of uniform aerial density and purity better than 99 9% was used as target. The data were recorded and analyzed using a 4K multichannel analyzer The present experimental Compton profiles of Sm constitute the first measurement. The results are compared with theoretical Hartree-Fock free-atom profiles

Keywords : Compton scattering, Compton profile, electron momentum density.

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1. Introduction

When radiation is Compton scattered from a body of electrons the emerging beam is Doppler-broadened because of the motion of the target electrons. The spectral analysis of the Compton scattered radiation reveals the line shape which according to impulse approximation, can be reduced to the 'Compton profile'. The impulse approximation assumes that the reaction time involved in the Compton scattering is so small that the initial and final electrons see the same constant potential. In the impulse approximation, the Compton profile $J(q)$ is the projection of the target's electron momentum distribution, $n(p)$, along the scattering vector axis, *i.e.*

$$J(q) = \iint n(p) dp_x dp_y . \quad (1)$$

Hence, it is used as a powerful tool for the investigation of electronic structure of materials, provided the impulse approximation remains valid [1–4]. This technique is particularly sensitive to the behaviour of the slowly moving outer electrons involved in bonding in condensed matter and serves as a reliable test of the accuracy of the calculated wave functions. Such basic information is useful in the study of all the physical properties of a system.

In this paper, we report a systematic study of the Compton profile of Sm. In Section 2, we briefly describe the experimental arrangement and results and discussion are given in Section 3.

2. Experimental details

The gamma ray spectrometer used in this work has been described elsewhere [5]. In the present work, Compton profiles of a thin foil of rare earth element Sm (purity better than 99.9%, $\mu t < 1$ [6]) were measured using an IGP Type Coaxial photon detector supplied by M/s. PRINCETON GAMMA-TECH, INC, NJ. It has dimensions of 5.05 cm of active diameter and 4.9 cm of active depth providing an active volume of 90 cc. The target atoms were excited using 59.54 keV gamma rays from 300 mCi Am-241 source. The optimum distance between the source and the scatterer was chosen to be 25 cm and that between the scatterer and detector, 25 cm. The gamma rays scattered at a mean angle 165° were detected by the IGP type detector having a resolution of 2 keV at 1332 keV and 780 eV at 122 keV. The linearity of the spectrometer was studied by using standard gamma ray sources and was found that it possesses very good linearity. The stability was also tested and it was

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observed that the shift in the peak channel was less than a channel over a period of 3 days. The data were collected and analyzed using a PC based 4K MCA. A separate measurement was made without the sample to obtain background contribution that was scaled to the measurement time of the foil and then subtracted point by point from the measured data. The signal to noise ratio was found to be 50 : 1. About 50000 counts were collected at the Compton peak. The raw data were corrected for background, absorption in the sample, instrumental resolution and differential scattering cross section [7,8]. The binding energy of *K* shell in Sm is greater than the recoil energy and hence these 1*s* electrons do not contribute to the Compton profile in the present measurements [9]. Hence, the experimental Compton profiles were normalized to the area of corresponding free-atom profile in the momentum range of 0 to 7 a.u. excluding the contribution of 1*s* electrons.

3. Results and discussion

The Compton profile of Sm was measured with the aid of experimental set up described in Section 2. The present experimental results for Sm are compared in Table 1 and Figure 1 with theoretical values calculated from the relativistic Hartree-Fock wave functions [10]. It can be seen that at

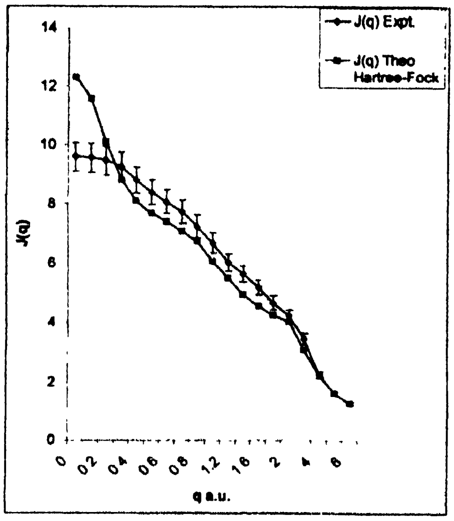

Figure 1. Comparison of the present results of Sm with theoretical values based on Hartree-Fock wave functions

Table 1. Comparison of Compton profile of Sm with theory.

q a.u.	$J_{(q)}$ Expt	$J_{(q)}$ Theo Hartree-Fock [10]
0.0	9.601	12.3
0 1	9 565	11 6
0.2	9 484	10 1
0 3	9 270	8 84
0.4	8 833	8.09
0.5	8.410	7 68
0.6	8.087	7 39
0.7	7.735	7 09
0.8	7.255	6.76
0.9	7.026	–
1.0	6.689	6.06
1.2	6.012	5.46
1.4	5.608	4 92
1.6	5.160	4.54
1.8	4.651	4.25
2.0	4.224	4.02
3 0	3.437	3.07
4.0	2.250	2.21
5.0	1.583	1 60
6 0	1.215	1.23
7.0	0.995	1.00

$q \doteq 0$ a.u., the measured values are smaller (~28%) than Hartree-Fock Compton profiles. It is due to the fact that the contribution of inner-core electrons is small in this region. Also, this deviation indicates the neglect of electron correlation beyond the HF parallel spin exchange. A proper inclusion of electron correlation produces an isotropic correction, which reduces the difference between experiment and theory. However, between 0.3 and 3.0 a.u., the present results are slightly broader than the theory. This broadening may be due to electron correlation, which pushes a part of the occupied states below the Fermi momentum to momentum values above the Fermi momentum. In the high momentum transfer region, $q > 3.0$ a.u., theoretical values are very close to the corresponding experimental data. It is known that the contribution of valence electron is very small in this region and hence, most of the contribution may be due to the inner-core electrons. These inner-core electrons are reasonably described by the free-atom values.

4. Conclusion

In this paper, we have reported experimental data on Compton profile of rare earth element Sm. The results are in relatively good agreement with Hartree-Fock Compton profile data particularly in the high momentum transfer region. In order to throw more light on the electron momentum distribution of rare earth elements, improvement in the calculations and more extensive and systematic measurements particularly with high-energy gamma ray photons are needed.

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