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The charge transfer in AgBr compound in terms of Compton profile and by adopting the ionic model

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Abstract

In this paper the Compton profile $J(p_z)$ for AgBr compound is calculated by using the superposition model and compared with available experimental value ,while the values of (Cp) $J(p_z)$ for the covsitituent namely Ag were taken from our previous study on AgCl to check whether there is any charge transfer between Ag metal and the Br , The Ionic model was applied for this purpose and found a fraction of charge is transfer from the d-state of the metal Ag to p-state of Br ,the best electron configuration for the AgBr compound is found to be Ag ($4d^{9.1}$ $5s^1$) Br($4s^2$ $4p^{5.1}$)

Key Word: Ionic model, Superposition model, RFA model, Compton profile (CP) $J(p_z)$,Free electron (FE) model ,Free atom (FA) model .

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1.Introduction

The inelastic Compton scattering is a sensible probe for investigating electronic structure of verity of materials ,the behavior of valence electrons of atoms .

The Compton technique is not sensitive to the sample purity , the lattice defects ,or to the surface and it samples the electrons in the crystal uniformly . Moreover ,Compton scattering is directly related to the electronic ground state and allows to extract the discontinuity in the electron momentum density associated with the fermi-surface topologies and electron correlation effects [1]. The Compton scattering experiment conduct three types of interactions between the X-ray or ɤ-ray photons and the atoms of the substance [2]. For the inelastic scattering ,the electron in the atom is considered free and static (bound electron), the photon give energy to the electron and the remaining energy of the photon is used to pump the photon in different direction and the overall momentum of the system remains preserved [3,4,5]. In order to get the photon to collide with the electron associated with the atom, the photon energy must be greater than the electron's energy. Compton observed that when the photon falls on the target material (electron) at a certain wavelength, the radius of the beam from the target material will change. The change depends on the angle (Ø) of the probe and does not depend on the target material of the falling beam[6]

2. Theory

2.1 (RFA,FE,FA) models

The calculated values of CP for Ag by using (RFA,FE,FA) models given else where [7], $J(p_z)$ for bromine (Br) element were taken directly form the tables of Biggs etal[8].

2.2 Super position model

To compute the $J(p_z)$ for AgBr compound , it is essential to use the values of $J(p_z)$ for Ag obtained by the three different models i.e . (RFA,FE and FA) and adding to them the values of Br separetly as in the equation [9]

$$J^{sup.}(p_z)=C\,J^{Ag}(p_z) + D\,J^{Br}(p_z)\text{…….(1)}$$

C and D represent the rational concentration . Also [10]

$J_{RFA}^{sup}(p_z)$=C $J_{RFA}^{Ag}(p_z)$ +D$J_{Biggs}^{Br}(p_z)$……(2)

$J_{FE}^{sup}(p_z)$=C $J_{FE}^{Ag}(p_z)$ +D$J_{Biggs}^{Br}(p_z)$…… (2)

$J_{FA}^{sup}(p_z)$=C $J_{FA}^{Ag}(p_z)$ +D$J_{Biggs}^{Br}(p_z)$…… (2)

All these values of J(p_z) for AgBr compound calculated by equation 1and 2 are given in table Experiment the values of reference [10] are included also

2.3 Ionic model

in order to find the best and favourable electronic arrangement achieved by any of the theoretical models mentioned earlier which must be more close to experimental values of reference [10] for AgBr compound , the computation based on the fact that the electrons supposed not to be in areal space but are located in the space of momentum , hence the talk will be about the electron momentum instead of speaking on the electron alone ,in this process the electrons cloud will surround the compound , we apply the ionic model to ensure if there are any transition of charge between the components of the AgBr compound , the experimental Compton profile values J(p_z) for silver (Ag) in [7] was used to obtain the valence electrons curve by subtracting these values from the core values which can be obtained directly from [8] then devided by the number of valence electrons ,we can express all these by the following equations:

J(p_z)exp .($1s^2 \rightarrow 4d^{10}$) –J(p_z)core ($s^2 \rightarrow 4p^6$)= J(p_z)valence.... (3)

J(p_z) for one valence electron=J(p_z)valence/10…..(4)

3. Results and Discussion

In table (1) we present all the calculated values of Compton profile for AgBr compound by applying the superposition model and compered all these with the available experimental values by ref .[10] ,all these values are normalized to the area under curve of free atom profile i.e (33.777) electron all the values given in table .1 are drawn in figure .1. To check which one among the various theoretical values are close to experimental values.

Comparing first the various values in the high momentum region (i.e.>2 a.u) it is seen that all theoretical values are nearly equal , this is so because in this region are the contribution of valence electrons are insignificant and only core electrons contribute , their values are almost the same in all models and have been obtained from free atom values ,interestingly these theoretical values are already very close to the experiment this once again confirms the fact that the inner electrons remain almost unaffected in the bond formation and the simple atomic model provides a reasonable description for these electrons. In order to investigate the we compare the various values in the low momentum region . It is seen that the RFA values (column 4) differ appreciably than other values .In figure .2 we plot the difference ΔJ(theory –experiment) for the various models obtained by the equation [11]

$$\sum_{p_z=6}^{7\ a.u} |\Delta J(Theo - EXP|^2 \ldots\ldots (5)$$

It turned out that Δ^2 was lowest for RFA model values and is closest to experimental values In order to obtain the best electronic order of a compound, the amount of charge transferred from the silver element to the bromine element is between ($0 \leq x \leq 1$). When transferring a charge (0.1) from the level of equivalence (4 d) of the silver atom to the level of equivalence (4p) we get the best electronic order of the silver bromide compound and the closest to the experiment results available to the compound Ag ($4d^{9.9}\ 5s^1$) Br ($4s^2\ 4p^{5.1}$) as given table .2.

4.Conclusions

It is concluded that RFA model is the best model for the study of the Compton curve of the silver bromide compound, where the results of this model are closer to the experimental values than the FA model as well as the FE model. Directly, the components of the compound are studied and the results are collected by superposition.

As for the ionic model, we notice that there is a transfer of the charge from the silver element to the bromine by 0.1 electron in the silver bromide compound.

Table 1. The theoretical values of the compound (AgBr) which were compared with the measured values of ref[10] and located in the momentum zone confined between (0-7 a.u.).

Pz (a.u.)	**J(Pz) (e/a.u.)**			
	Superposition model for AgBr			**Exp.[10]**
	Free Atom	Free electron	RFA	
0	15.38	14.7815	14.60007	**13.594**
0.1	15.17	14.71443	14.54433	**13.530**
0.2	14.62	14.50926	14.34945	**13.422**
0.3	13.93	14.13896	13.98709	**13.204**
0.4	13.23	13.56845	13.47231	**12.935**
0.5	12.55	12.92797	12.9085	**12.462**
0.6	11.9	12.13224	12.14711	**11.936**
0.7	11.27	11.27236	11.31656	**11.374**
0.8	10.66	10.36433	10.56633	**10.858**
1	9.54	9.521111	9.454606	**9.787**
1.2	8.56	8.549067	8.492562	**8.752**
1.4	7.74	7.723925	7.678079	**7.794**
1.6	7.01	7.00377	6.969304	**7.026**
1.8	6.38	6.376693	6.353735	**6.462**
2	5.82	5.815721	5.801359	**5.929**
3	3.86	3.86367	3.880527	**3.972**
4	2.78	2.782467	2.808189	**2.795**
5	2.102	2.102794	2.126623	**2.074**
6	1.623	1.63027	1.648288	**1.575**
7	1.27	1.270804	1.286062	**1.261**

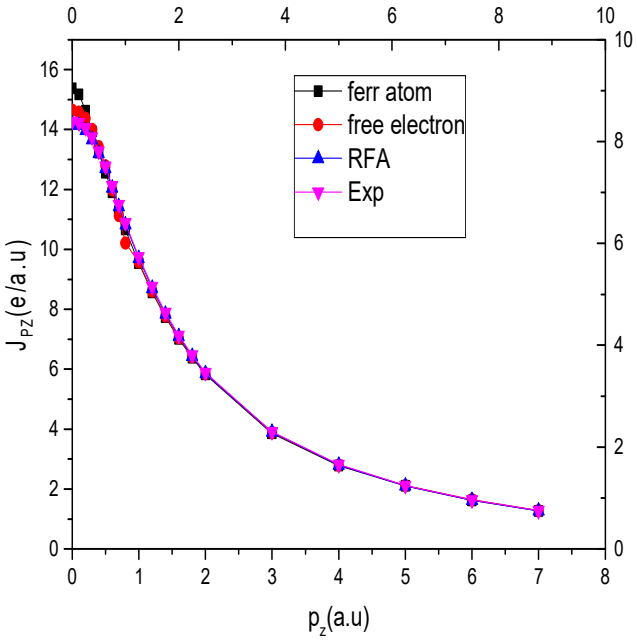

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Figure1.Comparison of various theoretical experimental values of ref [10]Compton curves with the AgBr in the momentum zone between(0-7 a.u)

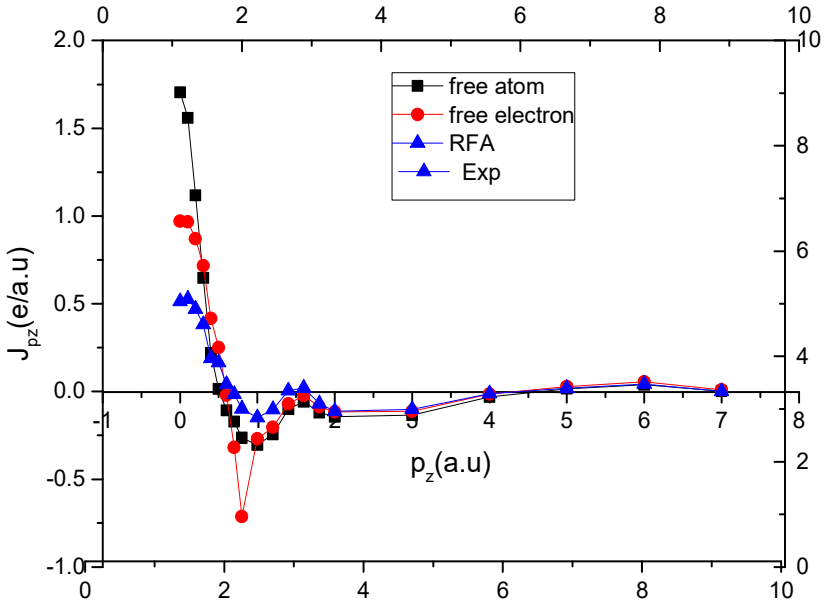

Figure 2. Curves of difference by applying $\sum \Delta^2$as given in the text for AgBr compound

Table2. J (p_z) values of the silver bromide compound calculated by the consideration of the charge transfer adopting the Ionic model

P_z(a.u)	$J(p_z)$(e/a.u)	Exp.AgBr[10]
	Ionic model	
	$Ag(4d^{9.9}5s^{1})Br(4s^{2}\ 4p^{5.1})$	
0	14.04157	**13.594**
0.1	13.97768	**13.530**
0.2	13.73494	**13.422**
0.3	13.29378	**13.204**
0.4	12.70874	**12.935**
0.5	12.05411	**12.462**
0.6	11.11857	**11.936**
0.7	10.39253	**11.374**
0.8	9.787123	**10.858**
1	8.670686	**9.787**
1.2	7.707249	**8.752**
1.4	6.893414	**7.794**
1.6	6.202958	**7.026**
1.8	5.610292	**6.462**
2	5.099778	**5.929**
3	3.406588	**3.972**
4	2.551846	**2.795**
5	2.001523	**2.074**
6	1.584076	**1.575**
7	1.244598	**1.261**

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