

Photon cross sections around K absorption edges

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Abstract : The mass attenuation coefficients of 13 elements at photon energies 5.895, 6.400 and 8.041 keV are determined accurately by employing a proportional counter. For elements Al, Cu, Mo, Ta and Pb elemental foils are used whereas for elements covering the range $16 \leq Z \leq 30$, the μ/ρ values are derived from their compounds. It is shown that the experimental values agree closely with the theoretical values of Saloman *et al* for those elements whose absorption edges are far away, on either sides of the absorption edge. But when the absorption edge is close to incident photon energy, that is between -1 keV to $+2$ keV, the μ/ρ values deviate significantly. The deviation in the post-edge region is attributed to such effects as XRS, EXAFS whereas in the pre-edge region it is attributed to RRCS/RRS.

Keywords : Photon cross sections, K -absorption edges, mass attenuation coefficients

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1. Introduction

It was shown earlier by us [1] that even by employing a proportional counter it is possible to obtain a unique and accurate value of the X-ray attenuation coefficient not only for element but also for compound. However, this would be possible when counting only those photons that are under the FWHM position of the full energy peak of the incident photons and considering only those thicknesses that lie in the transmission range (T), $0.5 \geq T \geq 0.25$. or $0.7 \leq \mu t \leq 1.4$.

2. Experiment and results

The incident X-ray beam is derived from radioactive source. The K_β component of the X-rays are filtered out by differential absorption technique, so that the incident beam consists essentially of K_α X-rays and other associated γ -rays, if any. The contribution from the radiations other than interested X-rays are estimated and the true counts are determined. The details of this procedure is given in one of our earlier papers [2]. The X-ray energies considered here are 5.895, 6.400 and 8.041 keV from ^{55}Fe , ^{57}Co and ^{66}Zn sources respectively. In order to check whether the incident X-ray beam essentially consists of K_α

components we have determined μ/ρ of elements using pure elemental foils of Al, Cu, Mo, Ta and Pb (Pb, only in the case of 8.041 keV X-rays). Only after ascertaining that our experimental values closely agrees with the recent theoretical values we proceeded to measure the μ/ρ values of the compounds. The details of the compounds are presented in Table 1. Thin, uniform foils of the compounds are prepared by depositing the aqueous solution of

Table 1. Details of the various compounds used in the present investigations

Chemical	Z*	K-shell binding energy [5]	Purity in %	Impurities present in %	Manufacturer
MgSO ₄ ·7H ₂ O	16	2 472	99	Not mentioned	B D.H., India
CaSO ₄ ·2H ₂ O	20	4 038	98	Fe-0.001, Cl-0.005 heavy metals-0.002	Aldrich, USA
NaVO ₃	23	5.465	97	Not mentioned	Fluka, Switzerland
Cr(C ₂ H ₃ O ₂) ₃ ·H ₂ O	24	5.989	99	Not mentioned	Aldrich, USA
MnSO ₄ ·H ₂ O	25	6.539	98	Cl-0.05, Zn-0.05, Fe-0.002, Pb 0.002	S D's Fine Chemicals, India
FeSO ₄ ·7H ₂ O	26	7 112	98	Cr-0.005, Zn-0.005, Mn-0.05	Aldrich, USA
Co(C ₂ H ₃ O ₂) ₂ ·4H ₂ O	27	7 709	99	Cl-0.005, Fe-0.02, NO ₃ -0.02, Ni-0.01, SO ₄ -0.01	Sarabhai Chemical, India
ZnSO ₄ ·7H ₂ O	30	9.659	99	Cl-0.002, Fe-0.005, Pb-0.002	S D's Fine Chemicals, India

Z* : Z of the relevant constituent element

these compounds on thin uniform good quality Whatman blotting paper. The uniformity is checked by X-ray transmission method by exposing a small portion of the foil at a time. Only those foils whose entire area was uniform were selected. The mass per unit area of these foils was found for each foil by weighing with a microbalance and then measuring the area using a travelling microscope. A known amount of solution prepared from a compound with known concentrations was then deposited uniformly on the selected filter paper foil. After evaporation, the uniformity of the sample foil was checked using the X-ray transmission method and only those foils whose entire area was uniform were selected, and then the mass per unit area of these foils was determined. The mass per unit area of the filter-paper was then subtracted to obtain the mass per unit area of the compound deposited on the foil. To obtain foils of higher mass per unit area, the concentration of the solution was increased and the procedure was repeated.

The μ/ρ values thus determined are presented in Tables 2, 3 and 4 for three energies for elements and compounds. The μ/ρ values of elements in the range $16 \leq Z \leq 30$ are derived from their respective compounds using the mixture rule using theoretical values of constituent elements except the interested one. Since all other constituent elements of these compounds are of low Z , the absorption edges of these elements are far away from the incident photon energies. Hence the theoretical values are not affected by the edge effects or chemical environment. So we can use the mixture rule, with the theoretical values of the constituent low- Z elements to calculate the μ/ρ of the interested element in the compound. Values calculated in this manner are given in Table 4 for three energies.

Table 2. Comparison of experimental and theoretical values of μ/ρ of various elements for 5.895, 6.400 and 8.041 keV X-rays.

Element	5.895 keV			6.400 keV			8.041 keV		
	Expt cm ² .g ⁻¹	Theo cm ² .g ⁻¹	P.D. %	Expt. cm ² .g ⁻¹	Theo cm ² .g ⁻¹	P.D. %	Expt. cm ² .g ⁻¹	Theo. cm ² .g ⁻¹	P.D. %
Al	121.5 ± 0.5	121.0	+ 0.4	96.2 ± 0.2	96.0	+ 0.2	50.5 ± 0.3	50.2	+ 0.4
Cu	120.7 ± 1.1	121.4	- 0.5	96.2 ± 0.6	95.8	+ 0.4	52.1 ± 0.5	53.0	- 1.7
Mn	350.0 ± 2.2	353.0	- 0.8	288.2 ± 2.5	284.3	+ 1.4	158.5 ± 0.8	154.6	+ 2.5
Ta	354.9 ± 1.5	353.2	+ 0.4	291.1 ± 2.9	286.0	+ 1.8	162.6 ± 1.0	161.6	+ 0.6
Pb	---			---			231.0 ± 1.0	226.1	+ 2.2

From Table 2, we see that our experimental values closely agree with the theoretical values. This confirms that the method we adopted, yield reliable and accurate values of μ/ρ . This also confirms that incident photon beam consists essentially of K_{α} component and whatever small quantity of K_{β} component present in the beam, is inconsequential and hence μ/ρ values correspond to K_{α} energy only.

In Table 3, we give the μ/ρ values for compounds at three photon energies. We see that the μ/ρ values for photon energies, far away from the absorption edges of the constituent elements are in close agreement with the theoretical values, whereas those in the region $- 1 \text{ keV} \leq \Delta E = (E_x - E_k) \leq + 2 \text{ keV}$, where E_x and E_k are the incident photon and K -absorption edge energies respectively, deviate from the theoretical values. The compounds which fall into this category are the compounds of vanadium, chromium and manganese at 5.895 and 6.400 keV, and the compounds of manganese, cobalt and iron at 8.041 keV.

Since the edge effects and chemical environment at and around the target atom affected the μ/ρ values of the target atom, we derive the μ/ρ value of each of the target atom from the

Table 3. Comparison of experimental and theoretical values of μ/ρ of various compounds for 5.895, 6.400 and 8.041 keV X-rays

Compound	5.895 keV			6.400 keV			8.041 keV		
	Expt. $\text{cm}^2\text{-g}^{-1}$	Theo. $\text{cm}^2\text{-g}^{-1}$	P.D. %	Expt. $\text{cm}^2\text{-g}^{-1}$	Theo. $\text{cm}^2\text{-g}^{-1}$	P.D. %	Expt. $\text{cm}^2\text{-g}^{-1}$	Theo. $\text{cm}^2\text{-g}^{-1}$	P.D. %
$\text{MgSO}_4 \cdot 7\text{H}_2\text{O}$	60.0 ± 0.8	59.6	+0.7	46.6 ± 0.8	47.1	+1.1	24.5 ± 0.1	24.3	+1.2
$\text{CaSO}_4 \cdot 2\text{H}_2\text{O}$	147.2 ± 2.0	148.5	-0.9	123.9 ± 1.3	123.9	+0.3	63.0 ± 1.6	63.2	-0.3
NaVO_3	180.0 ± 2.4	229.5	-21.6	192.6 ± 1.9	186.8	+3.0	100.2 ± 1.2	101.4	-1.2
$\text{Cr}(\text{C}_2\text{H}_3\text{O}_2)_3 \cdot \text{H}_2\text{O}$	43.0 ± 0.9	31.2	+37.9	103.4 ± 1.0	117.0	-11.6	59.0 ± 0.4	58.8	+0.3
$\text{MnSO}_4 \cdot \text{H}_2\text{O}$	75.3 ± 0.3	79.0	-4.6	71.0 ± 0.4	64.6	+9.9	96.4 ± 1.0	112.1	-14.0
$\text{FeSO}_4 \cdot 7\text{H}_2\text{O}$	62.0 ± 2.7	61.9	+0.2	49.7 ± 0.7	49.0	+1.9	71.6 ± 0.8	78.5	-8.8
$\text{Co}(\text{C}_2\text{H}_3\text{O}_2)_2 \cdot 4\text{H}_2\text{O}$	40.9 ± 0.7	40.5	+1.2	31.9 ± 0.6	32.0	-0.2	94.7 ± 0.5	82.7	+14.5
$\text{ZnSO}_4 \cdot 7\text{H}_2\text{O}$	73.4 ± 0.8	73.3	-0.2	58.6 ± 0.7	58.4	+0.3	31.4 ± 0.2	30.9	+1.6

Table 4. Comparison of experimental and theoretical values of μ/ρ of derived elements for 5.895, 6.400 and 8.041 keV X-rays.

Element	5.895 keV			6.400 keV			8.041 keV		
	Expt. $\text{cm}^2\text{-g}^{-1}$	Theo. $\text{cm}^2\text{-g}^{-1}$	P.D. %	Expt. $\text{cm}^2\text{-g}^{-1}$	Theo. $\text{cm}^2\text{-g}^{-1}$	P.D. %	Expt. $\text{cm}^2\text{-g}^{-1}$	Theo. $\text{cm}^2\text{-g}^{-1}$	P.D. %
S	224.7 ± 3.5	221.5	+1.4	175.0 ± 1.5	177.0	-1.1	94.7 ± 0.8	93.0	+1.8
Ca	385.2 ± 5.6	391.0	-1.5	336.8 ± 3.6	330.0	+2.1	168.7 ± 2.9	169.8	-0.6
V	370.7 ± 5.7	489.2	-24.2	411.8 ± 4.1	398.0	+3.5	220.3 ± 2.8	218.8	+0.7
Cr	125.6 ± 4.2	69.5	+80.8	429.5 ± 4.6	493.8	-13.0	249.5 ± 1.9	248.3	+0.5
Mn	61.8 ± 2.8	71.2	-13.3	81.6 ± 0.5	61.9	+31.9	225.6 ± 3.1	274.0	-17.7
Fe	89.6 ± 0.9	88.9	+0.7	71.5 ± 1.0	70.0	+2.1	279.0 ± 3.9	301.2	-7.4
Co	97.0 ± 2.4	98.2	+1.0	77.6 ± 1.5	78.0	-0.5	384.3 ± 2.0	320.9	+19.7
Zn	135.6 ± 3.5	135.1	+0.3	106.4 ± 1.3	108.0	-1.4	61.7 ± 0.8	59.5	+3.7

respective compound using the mixture rule. The values are given in Table 4, along with the theoretical values extracted from the Tables of Saloman *et al* [3]. From Table 4, we see clearly that the experimental values agree closely with the theoretical values for all those target elements whose absorption edges are far away from the incident photon energies. On the other hand, for those elements whose absorption edges lie in the region $-1 \text{ keV} \leq \Delta E \leq +2 \text{ keV}$ show deviation from the theoretical values. The positive sign indicates that E_i is greater than E_k and so corresponds to post-edge region and the negative sign indicates the pre-edge region. Also we see that the deviation is both positive and negative and the magnitude varies from 3.5% to 81%.

3. Discussion

The close agreement between the theoretical and the experimental μ/ρ values for elements confirms the validity of our method of determining the μ/ρ values. The maximum deviation of 2.5% observed in the case of Mo is expected as the theoretical values for high Z elements themselves are having 2 to 3% uncertainty.

In the case of compounds, the target atom is surrounded not only by the atoms of the same kind but also of different kinds. In addition, it is expected that the target atom will have edge structures extending upto 1 keV beyond the edge. So we may expect that the total photon cross section are affected by these effects, resulting in the deviation in measured μ/ρ values from that of theoretical values which are calculated for isolated atoms.

We see that in Tables 3 and 4, that measured values deviate from the theoretical values only when photon is close to the K-shell binding energy. The same compound yields μ/ρ value close to the theoretical value when photon energy is far away from its edge energy. This indicates two things, one is that the compound is pure enough and the other is that the edge effects are probably present along with the environmental effect. For example, let us take chromium compound. The K-edge energy of the chromium is 5.989 keV, it shows +81%, -13% and -0.5% when the photon energy is 5.895, 6.400 and 8.041 keV. If this compound has any impurity it would not have resulted in μ/ρ value which agrees closely with the theoretical values when its edge is far away from incident photon energy (that is at 8.041 keV). So the deviation observed at other energies are genuine and are due to edge effects. In the post-edge region the influence of effects such as XANES, EXAFS and XRS are well known. They exhibit oscillatory nature, resulting in positive and negative deviation of μ/ρ value. This can be seen in Table 4. So we can attribute part of deviation observed in the post-edge region to these effects and part to chemical environmental effect. Of course this is purely qualitative. In order to measure the chemical environmental effect quantitatively, we have to conduct measurements using elemental as well compound form of the same substance.

More important and interesting point is, in the pre-edge region also we observe the deviation in both ways. We can explain positive deviation by bringing in the Resonant Raman-Compton effect whose existence has recently been confirmed. But the negative

deviation in this region cannot be explained by any of the existing theories corresponding to pre-edge region, since the cross section can not become negative when any effect is present. However, an oscillatory nature of any effect can cause the values to go in both ways, similar to EXAFS in the post-edge region. Our results may be indicative of this, supporting the view expressed by Manninen *et al* [4] who predicted that there may be pre-edge structure similar to post-edge structure. However, much work in this direction is necessary to confirm these observations. Thus, we can conclude that the study of the photon interaction at and around absorption edge is very important both from fundamental as well as application points of view.

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