propafenon and butafenon. Suitable three-beam cases with almost equal intensities of the reflections involved were selected from a data set measured prior to the three-beam measurements. The structures were later solved by direct methods.

There is one essential point open for further investigation. We have stated in the preceding theoretical paper (Weckert & Hümmer, 1990) that in Laue–Laue and Laue–Bragg diffraction geometry *Pendellösung* effects occur. Then the energy flow into the primary diffracted beam depends on the thickness of the crystal plate and the ψ-scan profiles with constant triplet phase depend on the crystal dimensions. By averaging over the *Pendellösung* the phase information is lost. Experimental, we use non-cut crystals with grown faces, and the crystals are bathed by the incident beam. Therefore, the crystal thickness varies over the cross section of the diffracted beam. As a consequence, we guess that the *Pendellösung* effects are averaged out, so that the Laue–Laue and Laue–Bragg parts give no phase information. In addition, these are affected by anomalous absorption. Thus, we assume that only parts of the primary diffracted beam that are Bragg reflected carry the phase information.

In conclusion, the achievable accuracy of experimental triplet phase determination should be sufficient to solve structures that cannot be solved otherwise by a combination of measured triplet phases and direct methods.

These results were reported at the 11th European Crystallographic Meeting in Vienna (Weckert & Hümmer, 1988) and in part at the Fourteenth International Congress of Crystallography in Perth (Hümmer, Bondza & Weckert, 1987; Weckert, Bondza & Hümmer, 1987).

References

BERMAN, H. M. (1970). *Acta Cryst.* B26, 290–299.
BROWN, C. J. & SADANAGA, R. (1965). *Acta Cryst.* 18, 158–164.
BURZLAFF, H. (1988). Private communication.
HÜMMER, K. & BILLY, H. (1986). *Acta Cryst.* A42, 127–133.
HÜMMER, K., BONDZA, H. & WECKERT, E. (1987). *Acta Cryst.* A43, C222.
HÜMMER, K. & WECKERT, E. (1990). *Acta Cryst.* In the press.
HÜMMER, K., WECKERT, E. & BONDZA, H. (1989). *Acta Cryst.* A45, 182–187.
HVOSLEF, J. (1968). *Acta Cryst.* B24, 1431–1440.
KARTHA, G. & DE VRIES, A. (1961). *Nature (London)*, 192, 862–863.
LEHMANN, M. S. & NUNES, A. C. (1980). *Acta Cryst.* B36, 1621–1625.
PAULUS, E. F. (1988). Private communication.
SHEN, Q. & COLELLA, R. (1988). *Acta Cryst.* A44, 17–21.
TANG, M. T. & CHANG, S. L. (1988). *Acta Cryst.* A44, 1073–1078.
WECKERT, E. (1990a). In preparation.
WECKERT, E. (1990b). In preparation.
WECKERT, E. (1990c). In preparation.
WECKERT, E., BONDZA, H. & HÜMMER, K. (1987). *Acta Cryst.* A43, C264.
WECKERT, E. & HÜMMER, K. (1988). *Z. Kristallogr.* 185, 184.
WECKERT, E. & HÜMMER, K. (1990). *Acta Cryst.* A46, 387–393.

Problems Associated with the Measurement of X-ray Attenuation Coefficients. II. Carbon

Report on the International Union of Crystallography X-ray Attenuation Project

BY D. C. CREAGH

Department of Physics, University College, The University of New South Wales, Australian Defence Force Academy, Northcott Drive, Campbell, ACT 2600, Australia

AND J. H. HUBBELL

Center for Radiation Research, National Institute of Standards and Technology, Gaithersburg, MD 20899, USA

Abstract

Measurements are reported of the mass attenuation coefficient of carbon taken by laboratories participating in the International Union of Crystallography X-ray Attenuation Project. Data resulting from a similar study using silicon were published earlier [Creagh & Hubbell (1987). *Acta Cryst.* A43, 102–112]. The data are self consistent, for the most part, to 0·5% for the energy range 6 to 60 keV, and accords well

with earlier experimental data. These data are about 3% less than the theoretically calculated data [Saloman & Hubbell (1986). *X-ray Attenuation Coefficients (Total Cross Sections). Comparison of the Experimental Data Base with the Recommended Values of Henke and the Theoretical Values of Scofield from 0.1 to 100 keV.* Report NBSIR 86-3431. US Department of Commerce, NBS, Gaithersburg, MD, USA; Berger & Hubbell (1987). *XCOM. Photon Cross Sections on a Personal Computer.* Report NBSIR 87-3597. US Department of Commerce, Gaithersburg, MD, USA] over the energy range for which measurements were made. Hence carbon appears to be an example in which the renormalization, always a decrease, of Scofield's photo-effect calculations [Scofield (1973). Report UCRL-51236. Lawrence Livermore Laboratory, Livermore, California, USA], as was implemented by Hubbell [*Int. J. Appl. Radiat. Isot.* (1982), **33**, 1269–1290], would improve agreement with measured data.

1. Introduction

The International Union of Crystallography X-ray Attenuation Project was inaugurated by the Commission on Crystallographic Apparatus in 1979 as a response to widespread discontent among users of compilations of X-ray attenuation coefficients with the quality of data contained therein. It had as its principal aim the determination of which, if any, of the existing techniques for the measurement of X-ray attenuation coefficients could be relied upon to produce reliable data. A secondary aim was the evaluation of theoretical and semi-empirical compilations such as Scofield (1973), Cromer & Liberman (1970*a*, *b*), Storm & Israel (1970), Hubbell, Viegele, Briggs, Brown, Cromer & Howerton (1975), Hubbell, Gerstenberg & Saloman (1986) and Saloman & Hubbell (1986).

In the attempt of this project to achieve these aims three sets of specimen materials were sent to 25 laboratories worldwide for measurement. These materials were chosen because they posed well defined experimental problems which would test both experimental equipment and experimental technique. Materials chosen were

   (i) silicon – in the form of [111] or [110] cut dislocation-free float-zone rectangular parallelepipeds in which Laue–Bragg scatter can influence measurements significantly;

   (ii) carbon – in the form of pyrolytic graphite known to contain a relatively high density of voids, which would produce significant small-angle X-ray scatter;

   (iii) copper – in the form of thin highly rolled foils, which might produce significant scattering because of preferred orientation within the foils caused by the rolling process.

The silicon results have been reported by Creagh & Hubbell (1987). This paper is concerned with the evaluation of data for the carbon material measured by participants in the project, and by Creagh in separate parallel experiments using experimental procedures similar to those used by the participants in the project. This report will inter-compare the experimental data and then compare these data with the recent theoretical compilation of Saloman & Hubbell (1986), and the widely used photo-effect data of Cromer & Liberman (1970*a*, *b*) and Storm & Israel (1970). To these latter data must be added scattering contributions due to coherent and incoherent scattering processes using the results of Kissel, Roy & Pratt (1980), Hubbell & Øverbø (1979) and Hubbell *et al.* (1975). It is assumed here that the atomic scattering cross section σ may be adequately described by

$$\sigma = \sigma_{pe} + \sigma_R + \sigma_C \qquad (1)$$

where σ_{pe} is the photo-effect cross section; σ_R is the coherent (Rayleigh) scattering cross section; σ_C is the incoherent (Compton) scattering cross section.

Missing from (1) are cross sections for scattering processes such as nuclear Thomson scattering σ_N, Delbrück scattering σ_D and pair production σ_{pp}. These are negligibly small compared to σ for the range of photon energies reported here (6 to 60 keV).

2. Experimental procedure

In the first report on the International Union of Crystallography X-ray Attenuation Project, Creagh & Hubbell (1987) listed eight different configurations used by participants in the project. For carbon only five different configurations were used. These are shown schematically in Fig. 1. The number assigned to each configuration is the same as that in the paper on silicon.

Configuration [3] is similar to that described by Gerward (1983). This equipment was devised to measure the narrow-beam mass attenuation coefficient, μ/ρ, using the Beer–Lambert law

$$I = I_0 \exp\left[-(\mu/\rho)m_A\right] \qquad (2)$$

where I and I_0 are the beam intensities with and without the specimen and m_A is the mass per unit area of the absorber.

Slit-collimated X-rays emitted by a sealed X-ray tube were made monochromatic by diffraction from a perfect silicon crystal (220 or 440 reflection). The monochromatic beam was detected using an Si(Li) detector and the X-ray flux counted using a multichannel analyzer. The specimen was placed between the X-ray source and the monochromator with its surface perpendicular to the X-ray beam. So far as was possible, the specimen thickness was chosen such that $\ln(I_0/I)$ was close to 3, which is the optimum condition for the measurement of X-ray attenuation
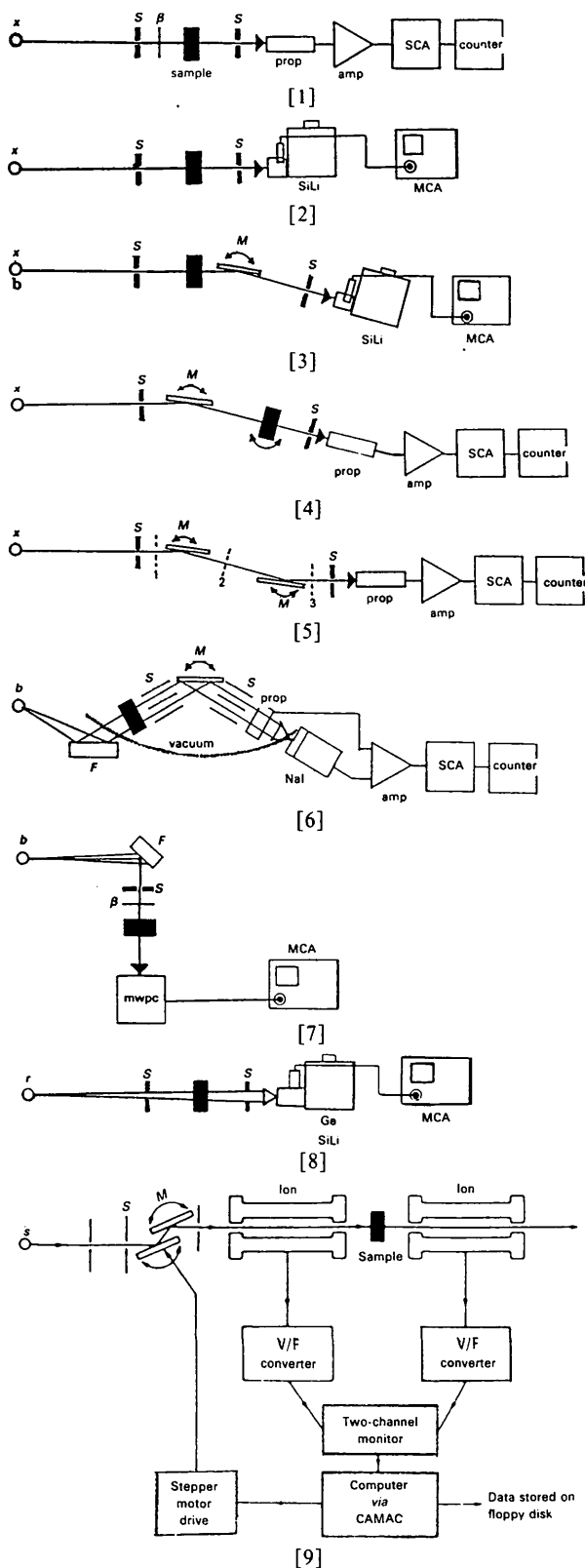
Fig. 1. Experimental configurations used by laboratories participating in the International Union of Crystallography X-ray Attenuation Project. The numbering on the diagram conforms to the numbering system in Creagh & Hubbell (1987).

coefficients (Nordfors, 1960). The apertures of the slit system could be varied so as to encompass the cone of small-angle X-ray scattering according to procedures suggested by Chipman (1955).

Because an energy dispersive system of high resolution (typically 160 eV) was used to detect the radiation all harmonics of the wanted radiation could be completely eliminated. The use of pile-up rejection together with the use of the region-of-interest facility within the multi-channel analyzer in conjunction with its live-time clock almost completely eliminated the need for dead-time corrections. Nevertheless the incident flux I_0 was varied and if any count-rate dependence was observed in the measurement of (μ/ρ), the true value was determined by extrapolating these measurements to zero count rate.

Configuration [4] is essentially the same configuration as that described by Calvert, Killean & Mathieson (1975) and Berry & Lawrence (1979). The radiation emitted from a sealed X-ray tube was made monochromatic by Bragg reflection from a silicon [111]-oriented perfect single crystal or a lithium fluoride [200]-oriented single crystal. The latter had a much greater mosaic spread than the silicon. The monochromatic beam could then pass through the sample, thence to a beam-defining slit and a proportional detector, the output of which passed through a preamplifier, amplifier and single-channel analyzer to a counter. Conventional dead-time techniques (Bertin, 1975) were employed in the analysis of the data. The most significant difference between this technique and that of configuration [3] is the fact that the specimen is tilted with respect to the incident beam so as to alter the effective thickness of the specimen.

Configuration [6] is similar to the configuration frequently used by X-ray fluorescence spectroscopists to determine the average attenuation coefficients for the purposes of making matrix corrections. It is different, however, from the usual arrangement in that the sample was placed between the material F, which emits its characteristic fluorescence lines when irradiated by the X-ray Bremsstrahlung emitted by a sealed X-ray tube (usually with a tungsten anode), and the monochromator crystal. The sample was placed within the vacuum chamber. Detection was by means of a proportional detector or scintillation detector which was followed by a counting chain which includes a single-channel analyzer to eliminate the contribution from unwanted X-ray photons. The deficiencies of the technique commonly used by X-ray fluorescence spectroscopists (sample placed in front of the scintillation counter, outside the vacuum chamber) have been described by Creagh (1976).

Configuration [7] is similar in principle to configuration [6] except that a novel multi-wire proportional counter (Hribar, Kodre, Moljk & Pahor, 1973) was used in conjunction with a multi-channel analyzer to

provide the necessary energy discrimination. Conventional dead-time corrections were employed.

Configuration [8] is typical of many systems used for low-energy nuclear radiation interaction cross-section measurements. The γ-ray source for these measurements was ^{241}Am, radiation from which was collimated by slits and passed through the sample, through scatter slits, and into a solid-state detector [either intrinsic germanium or Si(Li)]. The output from the detector was analyzed using a multi-channel analyzer. Conventional dead-time corrections were applied. The surface of the sample was placed normal to the incident beam.

Before considering the data produced by these very different configurations it is necessary to describe briefly the properties of the carbon samples used in this experiment. The samples were taken from a stock of POCO graphite donated by Poco Graphite Inc., Texas, USA. Sheets of POCO graphite ranging in thickness from 0·127 to 1·016 mm were cut into 15 mm squares. Each participant in the project was given about ten different thicknesses of sample.

The density of each sheet was determined prior to cutting and a value of 1·800 (5) g cm^{-3} was found. An essential part of this project was the measurement of the density of the specimens by participating laboratories. However, some laboratories did not measure the true density; rather they used the X-ray density tabulated in *International Tables for X-ray Crystallography* (1962), 2·266 g cm^{-3}.

The discrepancy in densities is due to the presence of voids within the graphite, and these voids give rise to small-angle X-ray scattering (SAXS). A detailed analysis of the SAXS from these POCO graphite samples will be presented for publication at a later date (Creagh & Henderson, 1990). Suffice to say that the Porod plots for all thicknesses of specimens yielded exponents of about −3·60 and analysis of the SAXS data indicated the average size of a void was 14 (1) Å. The SAXS is confined to a cone of half angle less than 6'. Laue photography failed to show any crystalline structure.

In summary the material is truly amorphous and it contains a high density of voids which are rather uniform in size.

If accurate results are to be obtained it is essential that these characteristics of the sample be taken into account in the design of the experimental equipment.

3. Results

The experimentally determined X-ray attenuation coefficient contains contributions from a variety of interactions of the X-ray beam with the sample material. The principal absorption and scattering cross sections, photo-effect (σ_{pe}), coherent (σ_R) and incoherent (σ_C), are assumed to add together to pro-

Table 1. *Values of the mass attenuation coefficient (μ/ρ) obtained by participants in the International Union of Crystallography X-ray Attenuation Project tabulated as a function of photon energy*

Values in *italics* were measured by participants in the project. Values in **bold type** were taken by Creagh. Values in normal type were taken by Gerward (1983). Units are cm^2 g^{-1}.

Line	Energy (keV)	Experimental configuration				
		3	4	6	7	8
Fe$K\alpha_1$	6·40384	8·731		8·738	8·656	
		8·771				
		8·733				
Co $K\alpha_1$	6·93032	6·810				
		6·811				
Fe $K\beta$	7·05198	6·481				
		6·478				
		6·483				
Co $K\beta$	7·64943	5·06				
		5·06				
Cu $K\alpha_1$	8·04778	4·344		4·51		
		4·350	*4·334*	4·344	*4·40*	
		4·334		4·239		
Cu $K\beta$	8·90520	3·221				
		3·222				
γ	14·0					*0·918*
γ	17·0					*0·598*
Mo $K\alpha_1$	17·477934	0·562	*0·567*	0·563		*0·593*
		0·561				
		0·561				
Mo $K\beta$	19·6083	0·450				
		0·450	*0·444*			
X-ray	40·06	*0·198*				
γ	59·5					*0·172*
						0·171

duce a total interaction cross section (σ) as shown in (1). An experimentalist can devise strategies to minimize one or another of these interaction cross sections, but in general he has little control over the data which ensue from his experiment.

In this particular experiment it is possible to ensure that all the coherent scattering produced by the voids is collected by the detector by following the procedure devised by Chipman (1955). This involves increasing the angular divergence of the collimating slit until the value of (μ/ρ) reaches its lowest value. In this way one can be confident that all the cooperative Rayleigh scattering due to voids enters the counter.

In Table 1 values of the mass attenuation coefficient (μ/ρ) obtained by participants in the International Union of Crystallography X-ray Attenuation Project are tabulated as a function of photon energy. For configuration [3] the values for (μ/ρ) for each of the listed energies agree with one another to better than 0·5%. The values of (μ/ρ) using X-ray sources without diffraction monochromatization are, however, sometimes significantly at variance with the results using configuration [3]. If one considers the photon energy 8·04778 keV which corresponds to the emission wavelength of Cu $K\alpha_1$, configuration [4] gives a slightly low value, whereas configuration

[6] gives one correct, one very low and one very high value. Configuration [7] gives a value which is 1% high.

For a photon energy of 17·47934 keV (Mo $K\alpha_1$) configuration [4] gives a value 1% higher than configuration [3] whereas configuration [8] gives a value 6% higher than configuration [3].

In general, however, most of the data are consistent to better than 0·5% precision. It must be commented however that some of the data have been recalculated because some participants used an incorrect value for the density of the carbon samples.

The next question to be answered concerns how well these data agree with the theoretically predicted values. Fig. 2 plots the contributions to the mass attenuation coefficient due to Rayleigh and Compton scattering and photo-effect absorption as a function of photon energy. The total mass attenuation coefficient is also plotted, together with the experimental data points. The theoretical values are taken from the most recent compilation by Saloman & Hubbell (1986) which uses recent photo-effect calculations by Scofield together with Compton-effect and Rayleigh scattering data contained in Hubbell & Øverbø (1979) and Hubbell *et al.* (1975).

The Compton scattered contribution almost doubles in magnitude as the energy increases and at higher energies is the dominant scattering mechanism. At higher energies still, Delbrück and nuclear Thomson scattering and pair production become significant but for the photon range relevant to this study they contribute an insignificant amount to the mass attenuation (or absorption) coefficient.

The Rayleigh scattering contribution drops by a factor of 6 for the same range of photon energies.

For lower photon energies the photo-effect contribution dominates the total interaction cross section. For high photon energies the Compton effect dominates the total interaction cross section. The effect of the voids on the scattering by the sample is reduced significantly as the photon energy increases.

On the scale of Fig. 1, agreement between theory and experiment appears to be excellent. There exists, however, a systematic difference between theory and experiment. In Table 2, the best experimental data are compared with the corresponding data from Saloman & Hubbell (1986) and Berger & Hubbell (1987) which enables interpolations to be made between theoretically determined data points. The theoretical data points are systematically larger than the experimental data points by between 2% for the photons of energy 6·40384 keV and 3% for the photons of energy 59·5 keV.

Given that the experimental values shown in Table 2 are in excellent agreement with other experimental values (Millar & Greening, 1974; Batterman, 1958; Bearden, 1966) we are led to conclude that they represent the true values of the mass attenuation

Table 2. *Comparison of the experimentally determined values of the mass attenuation coefficient (μ/ρ) with theoretically predicted values taken from Saloman & Hubbell (1986) and Berger & Hubbell (1987)*

Line	Energy (keV)	Experimental result	Theoretical result
Fe $K\alpha_1$	6·40384	8·733	8·97
Co $K\alpha_1$	6·93032	6·811	7·06
Fe $K\beta$	7·05198	6·481	6·68
Co $K\beta$	7·64943	5·06	5·24
Cu $K\alpha_1$	8·04778	4·344	4·50
Cu $K\beta$	8·90529	3·222	3·33
γ	14·0	0·918	0·955
γ	17·0	0·598	0·608
Mo $K\alpha_1$	17·47934	0·561	0·574
Mo $K\beta$	19·6083	0·450	0·458
X-ray	40·06	0·198	0·207
γ	59·5	0·171	0·176

coefficients. This implies, therefore, that systematic errors exist in the theoretical calculations on which the compilation of Saloman & Hubbell (1986) is based.

Parker & Pratt (1982) and Schaupp, Schumacher, Smend, Rullhusen & Hubbell (1983) have shown that there is little to choose between the modern relativistic treatments of Rayleigh scattering. Furthermore, Creagh (1988) has shown that very substantial agreement exists between the measured and the theoretical values of Rayleigh scattering cross sections. Reference to Fig. 2 shows that Rayleigh scattering contributes about 3% to the total interaction cross section at 6·40384 keV and 15% to the total interaction cross section at 19·6083 keV. At 59·5 keV the contribution to the total interaction cross section falls to about 5%. It must be expected, therefore, that errors in calculating the Rayleigh scattering cross section will make a relatively small contribution to the total interaction cross section.

Although some problems exist in the calculation of Compton scattering cross sections for condensed matter, Schumacher (1985) has shown that the compilation of Hubbell *et al.* (1975) remains the most
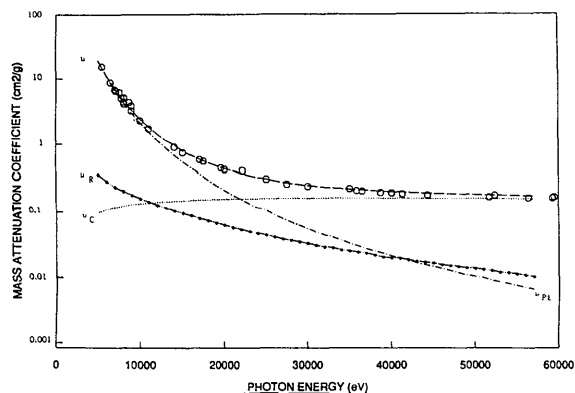

Fig. 2. Theoretical values of the photo-effect (μ_{pe}), elastic (μ_R) and inelastic (μ_C) mass attenuation coefficients plotted as a function of photon energy for carbon. The open circles represent experimentally determined values (Saloman & Hubbell, 1986).

Table 3. Comparison of the theoretical photo-effect mass attenuation coefficients

Listed are the photo-effect calculations of (μ/ρ) of Scofield (1973) (Sc), Cromer & Liberman (1970a, b) (CL) and Storm & Israel (1970) (SI). The Scofield (1986) values are larger than the others. Units are cm^2 g^{-1}.

Line	Energy (keV)	Scofield (1986)	Sc	CL	SI
Fe $K\alpha_1$	6·40384	8·59	3	5	7
Co $K\alpha_1$	6·93032	6·69	4	5	4
Fe $K\beta$	7·05198	6·32	4	5	4
Co $K\beta$	7·64943	4·89	4	6	5
Cu $K\alpha_1$	8·04778	4·16	4	6	6
Cu $K\beta$	8·90529	3·01	4	5	6
γ	14·0	0·699	4	5	6
γ	17·0	0·371	4	5	6
Mo $K\alpha_1$	17·47934	0·339	3	4	6
Mo $K\beta$	19·6083	0·232	3	4	4
X-ray	40·06	0·0218	5	6	6
γ	59·5	0·006	10	12	12

The column header group is "% deviation from Scofield (1986)" spanning Sc, CL, SI; the overall grouping is "Theoretical photo-effect mass attenuation coefficients".

reliable compilation for the Compton scattering cross sections. Since this cross section contributes strongly to the total cross section at high energies, significant errors can result from incorrect computational techniques. At a photon energy of 6·40384 keV the Compton scattering cross section is about 1% of the total interaction cross section, whereas at 59·5 keV it accounts for 91% of the total interaction cross section. Errors in the calculation of σ_C contribute significantly to the total cross section σ. In their evaluation of the existing cross section, Saloman & Hubbell (1986) have shown that the existing experimental data lie within 5% of the theoretical data over the range 50 to 100 keV, a region where σ_C is very much the dominant interaction mechanism. This suggests that there exists no major source of error in the calculation of σ_C.

Finally, the dominant mechanism for photon interaction over much of the range of photon energies is the photo-effect cross section σ_{pe}. It is of greatest significance for photons at the lowest energies in the range and becomes relatively insignificant for the highest energies in the range. The most recent compilation, that of Saloman & Hubbell (1986), presents the original (not renormalized) Scofield (1973) theoretical calculations, and it is with values taken from this compilation that the experimental results are compared in Table 2. The decision to make this comparison is based on the fact that the program *XCOM* [produced by Berger & Hubbell (1987) and based on the several compilations in Saloman & Hubbell (1986)] has been distributed widely to users of personal computers, and will ultimately be used by equipment manufacturers such as those engaged in the manufacture of equipment for X-ray fluorescence spectroscopy, electron probe microanalysis, X-ray diffraction *etc.* It is of some importance that scientists

understand the limitations of data they use on a day-to-day basis, the more so if these data are buried in the software of their computer system.

Table 3 gives the theoretical calculations of the mass attenuation coefficients related to the photo-effect cross sections by Scofield (1986) and the deviations from those values by the calculations of Scofield (1973), Cromer & Liberman (1970a, b) and Storm & Israel (1970). These deviations, [(μ/ρ) (Scofield, 1986)]$-$[(μ/ρ) X], where X represents the other compiled values, are expressed as a percentage of the Scofield (1986) value. Interpolation procedures have been used where no compiled values exist. Note that significant agreement exists between the three earlier compilations and they differ from the Scofield (1986) values quite significantly for low photon energies. Typically they are 3 to 5% smaller over the whole range of energies of Tables 1, 2 and 3. In fact they accord better with the experimental data than the Scofield (1986) data.

Whilst this indicates that, for carbon, the renormalization process has caused some improvement in the theoretical calculation, it does not follow that a similar situation exists for other atoms and other photon energies. Rather, this is one set of data within a large number of data sets which Hubbell, Gerstenberg & Saloman (1986) have evaluated and for which deviations between experiment and theory are recorded. The procedure they adopted is, on average, best for all elements and the whole gamut of photon energies.

In summary, one can say that the discrepancy between theory and experiment for carbon can be almost completely accounted for by an overestimation of the photo-effect cross section by the non-renormalized original Scofield cross-section formalism. Thus carbon appears to be one of the exceptions from the general tendency, noted by Saloman & Hubbell (1986), for the renormalized Scofield (1973) values, as provided by Hubbell (1982), to underestimate the photo-effect cross section. In a recent paper, Gerward (1989) suggests that the Scofield theoretical values with and without the Hartree–Slater to Hartree–Fock renormalization can be used as lower and upper limits of the experimental photo-effect cross sections. This suggestion would appear to have considerable merit.

4. Concluding remarks

A definitive set of experimental measurements of the mass attenuation coefficients of carbon for the photon energy range 6 to 60 keV has been produced. Of the measurements, those using experimental configuration [3], recommended by Creagh & Hubbell (1987) as the most reliable technique for measuring X-ray attenuation coefficients, agree with one another to better than 0·5% for the entire range of photon energies. The agreement between measurements made

with the whole range of experimental techniques is better than 1%.

These experimental results have been compared with the most recent theoretical compilations (Salo-man & Hubbell, 1986; Berger & Hubbell, 1987) and to three earlier compilations. It has been demonstrated that the experimental results are lower by 3 to 5% than the data in these tables. This can be attributed almost entirely to an overestimate in the photo-effect cross section for carbon by not using the re-normalization procedure prescribed by Scofield (1973) and implemented by Hubbell (1982). It must be stressed that whilst this problem has occurred for carbon it may not occur for other elements in the data tables.

It is imperative that scientists realize that it is essential that the characteristics of a sample be understood thoroughly before devising their experimental apparatus. Scientists must also realize that theoretically produced data tables may contain systematic errors.

APPENDIX
Participants who have provided data for the International Union of Crystallography X-ray Attenuation Project

CHAUDHURI, N. Department of Physics, University of North Bengal-PO Dt. Darjeeling, West Bengal, India PIN-734430.

CREAGH, D. C. Department of Physics, Royal Military College, Duntroon, ACT 2600, Australia.

DEL GRANDE, N. K. Lawrence Livermore National Laboratory, PO Box 808, Livermore, California 94550, USA.

GERWARD, L. Laboratory of Applied Physics III, Technical University of Denmark, Building 307, DK-2800 Lyngby, Denmark.

HARRIS, L. S. AND McCUAIG, N. Department of Physics, University of Surrey, Guildford, Surrey GU2 5XH, England.

KODRE, A., HRIBAR, M. AND AJLEC, B. Department of Physics, J. Stefan Institute, University of E. Kardelj, YU-61001 Ljubljana, Yugoslavia.

LAWRENCE, J. L. Department of Physics, University of St. Andrews, North Haugh, St. Andrews KY16 9SS, Scotland.

MEHROTRA, B. N. School of Physics, Universiti Sains Malaysia, Minden, Penang, Malaysia.

MIKA, J. F. AND MARTIN, L. J. Australian Radiation Laboratory, Lower Plenty Road, Yallambie, Victoria 3085, Australia.

NORRISH, K., HANCOCK, G. AND ROGERS, P. CSIRO Division of Soils, Urrbrae, Adelaide, South Australia.

O'CONNOR, B. School of Physics and Geosciences, WA Institute of Technology, Kent Street, Bentley, WA 6102, Australia.

UNO, R. Department of Physics, College of Humanities and Sciences, 3-25-40 Sakurajosni Setagaya-Ku, Tokyo, Japan.

References

BATTERMAN, B. W. (1958). Rev. Sci. Instrum. 29, 1132.

BEARDEN, A. J. (1966). J. Appl. Phys. 37, 1681-1692.

BERGER, M. J. & HUBBELL J. H. (1987). XCOM. Photon Cross Sections on a Personal Computer. Report NBSIR 87-3597. US Department of Commerce, Gaithersburg, MD, USA.

BERRY, A. A. & LAWRENCE, J. L. (1979). Acta Cryst. A35, 316-318.

BERTIN, E. P. (1975). Principles and Practice of X-ray Spectrometric Analysis, 2nd ed. New York: Plenum.

CALVERT, L. D., KILLEAN, R. C. G. & MATHIESON, A. McL. (1975). Acta Cryst. A31, 855-856.

CHIPMAN, D. R. (1955). J. Appl. Phys. 26, 1387.

CREAGH, D. C. (1976). J. Phys. E, 9, 88-90.

CREAGH, D. C. (1988). Aust. J. Phys. 38, 371-408.

CREAGH, D. C. & HENDERSON, S. (1990). To be submitted.

CREAGH, D. C. & HUBBELL, J. H. (1987). Acta Cryst. A43, 102-112.

CROMER, D. T. & LIBERMAN, D. (1970a). J. Chem. Phys. 53, 1891-1898.

CROMER, D. T. & LIBERMAN, D. (1970b). Report LA-4403. Los Alamos Scientific Laboratory, Los Alamos, NM, USA.

GERWARD, L. (1983). Acta Cryst. A39, 322-325.

GERWARD, L. (1989). J. Phys. B, 22, 1963-1969.

HRIBAR, M., KODRE, A., MOLJK, A. & PAHOR, J. (1973). Fizika (Zagreb), 5, 171-177.

HUBBELL, J. H. (1982). Int. J. Appl. Radiat. Isot. 33, 1269-1290.

HUBBELL, J. H., GERSTENBERG, H. M. & SALOMAN, E. B. (1986). Bibliography of Photon Total Cross Section (Attenuation Coefficient). Measurements 10 eV to 13·5 GeV. Report NBSIR 86-3416. US Department of Commerce, NBS, Gaithersburg, MD, USA.

HUBBELL, J. H. & ØVERBØ, I. (1979). J. Phys. Chem. Ref. Data, 8, 69-105.

HUBBELL, J. H., VEIGELE, H. L., BRIGGS, E. A., BROWN, R. T., CROMER, D. T. & HOWERTON, R. J. (1975). J. Phys. Chem. Ref. Data, 4, 471-538.

International Tables for X-ray Crystallography (1962). Vol. III. Birmingham: Kynoch Press. (Present distributor Kluwer Academic Publishers, Dordrecht.)

KISSELL, L., ROY, S. C. & PRATT, R. H. (1980). Phys. Rev. A, 22, 1970-2004.

MILLAR, R. H. & GREENING, J. R. (1974). J. Phys. B, 7, 2332-2344, 2345-2354.

NORDFORS, B. (1960). Ark. Fys. 18, 37-47.

PARKER, J. C. & PRATT, R. H. (1982). Research Report PITT-286. Univ. of Pittsburgh, PA, USA.

SALOMAN, E. B. & HUBBELL, J. H. (1986). X-ray Attenuation Coefficients (Total Cross Sections). Comparison of the Experimental Data Base with the Recommended Values of Henke and the Theoretical Values of Scofield from 0.1 to 100 keV. Report NBSIR 86-3431. US Department of Commerce, NBS, Gaithersburg, MD, USA.

SCHAUPP, D., SCHUMACHER, M., SMEND, F., RULLHUSEN, P. & HUBBELL, J. H. (1983). J. Phys. Chem. Ref. Data, 12, 467-512.

SCHUMACHER, M. (1985). Workshop on New Directions in X-ray Scattering.

SCOFIELD, J. H. (1973). Report UCRL-51236. Lawrence Livermore Laboratory, Livermore, California, USA.

SCOFIELD, J. H. (1986). Cited in X-ray Attenuation Coefficients (Total Cross Sections). Comparison of the Experimental Data Base with the Recommended Values of Henke and the Theoretical Values of Scofield from 0·1 to 100 keV. Report NBSIR 86-3431. US Department of Commerce, NBS, Gaithersburg, MD, USA.

STORM, E. & ISRAEL, H. I. (1970). Nucl. Data Tables, A7, 565-681.