Table 4.2.4.2. *Total photon interaction cross section (barns/atom) (cont.)*

| Radiation | Energy (MeV) | 97 Berkelium | 98 Californium |
|---|---|---|---|
| Ag $K\beta_1$ | 2.494E−02 | 2.13E+04 | 3.06E+04 |
| Pd $K\beta_1$ | 2.382E−02 | 2.18E+04 | 3.44E+04 |
| Rh $K\beta_1$ | 2.272E−02 | 2.41E+04 | 3.86E+04 |
| Ag $K\bar{\alpha}$ | 2.210E−02 | 2.50E+04 | 2.89E+04 |
| Pd $K\bar{\alpha}$ | 2.112E−02 | 2.98E+04 | 4.62E+04 |
| Rh $K\bar{\alpha}$ | 2.017E−02 | 3.37E+04 | 5.21E+04 |
| Mo $K\beta_1$ | 1.961E−02 | 3.64E+04 | 5.59E+04 |
| Mo $K\bar{\alpha}$ | 1.744E−02 | 2.01E+04 | 2.09E+04 |
| Zn $K\beta_1$ | 9.572E−03 | 7.63E+04 | 8.67E+04 |
| Cu $K\beta_1$ | 8.905E−03 | 9.27E+04 | 1.04E+04 |
| Zn $K\bar{\alpha}$ | 8.631E−03 | 1.01E+05 | 1.13E+05 |
| Ni $K\beta_1$ | 8.265E−03 | 1.13E+05 | 1.26E+05 |
| Cu $K\bar{\alpha}$ | 8.041E−03 | 1.43E+05 | 1.50E+05 |
| Co $K\beta_1$ | 7.649E−03 | 1.46E+05 | 1.52E+05 |
| Ni $K\bar{\alpha}$ | 7.472E−03 | 1.48E+05 | 1.61E+05 |
| Fe $K\beta_1$ | 7.058E−03 | 1.73E+05 | 1.87E+05 |
| Co $K\bar{\alpha}$ | 6.925E−03 | 1.82E+05 | 1.96E+05 |
| Mn $K\beta_1$ | 6.490E−03 | 2.16E+05 | 2.30E+05 |
| Fe $K\bar{\alpha}$ | 6.400E−03 | 2.43E+05 | 2.53E+05 |
| Cr $K\beta_1$ | 5.947E−03 | 2.72E+05 | 2.86E+05 |
| Mn $K\bar{\alpha}$ | 5.895E−03 | 2.78E+05 | 2.93E+05 |
| Cr $K\bar{\alpha}$ | 5.412E−03 | 3.49E+05 | 3.63E+05 |
| Ti $K\beta_1$ | 4.932E−03 | 4.47E+05 | 4.59E+05 |
| Ti $K\bar{\alpha}$ | 4.509E−03 | 4.26E+05 | 4.38E+05 |

This equation is not in a convenient form for computation and the alternative formalism presented by Sano, Ohtaka & Ohtsuki (1969) is often used in calculations. In this formalism,

$$\sigma_{\rm TD} = 2\pi r_e^2 \int_{-1}^{1} C_p f^2(q, Z)\{1 - \exp[-2M(q)]\}\, {\rm d}(\cos\varphi). \tag{4.2.4.9}$$

The values of $f(q, Z)$ are those of Cromer & Waber (1974).

Cross sections calculated using equation (4.2.4.8) tend to oscillate at low energy and this corresponds to the inclusion of Bragg peaks in the summation or integration. Eventually, these oscillations abate and $\sigma_{\rm TD}$ becomes a smoothly varying function of energy.

Creagh & Hubbell (1987) and Creagh (1987) have stressed that, before cross sections are calculated for a given ensemble of atoms, care should be taken to ascertain whether single-atom or single-crystal scattering is appropriate for that ensemble.

#### 4.2.4.2.3. *Theoretical Compton scattering data: $\sigma_C$*

The bound-electron Compton scattering cross section is given by

$$\begin{aligned}\sigma_C = \pi r_e^2 \int_{-1}^{1} &[1 + k(1 - \cos\varphi)]^{-2} \\ &\times \{+\cos^2\varphi + k^2(1 - \cos\varphi)^2 \\ &\times [1 + k(1 - \cos\varphi)]^{-1}\} I(q, z)\, {\rm d}(\cos\varphi).\end{aligned} \tag{4.2.4.10}$$

Here $k = \hbar\omega/mc^2$ and $I(q, z)$ is the incoherent scattering intensity expressed in electron units. The other symbols have the meanings defined in §§4.2.4.2.1 and 4.2.4.2.2.

Values of $\sigma_C$ incorporated into the tables of total cross section $\sigma$ have been computed using the incoherent scattering intensities from the tabulation by Hubbell *et al.* (1975) based on the calculations by Cromer & Mann (1967) and Cromer (1969).

### 4.2.4.3. *Comparison between theoretical and experimental data sets*

Saloman & Hubbell (1986) and Saloman *et al.* (1988) have published an extensive comparison of the experimental database with the theoretical values of Scofield (1973, 1986) for photon energies between 0.1 and 100 keV. Some examples taken from Saloman & Hubbell (1986) are shown in Figs. 4.2.4.1, 4.2.4.2, and 4.2.4.3.

Comparisons between theory and experiment exist for about 80 elements and space does not permit reproduction of all the available information. This information has been summarized in Fig. 4.2.4.4. Superimposed on the Periodic Table of the elements are two sets of data. The upper set corresponds to the average percent deviation between experiment and theory for the photon energy range 10 to 100 keV. The lower set corresponds to the average percent deviation between experiment and theory for the photon energy range 1 to 10 keV. An upwards pointing arrow $\uparrow$ means that $(\sigma_{\rm exp} - \sigma_{\rm theor}) > 0$. No arrow implies that $(\sigma_{\rm exp} - \sigma_{\rm theor}) = 0$. A downwards pointing arrow $\downarrow$ means that $(\sigma_{\rm exp} - \sigma_{\rm theor}) < 0$. An asterisk means no experimental data set was available.

For example: for tin ($Z = 50$), the experimental data are on average 5% higher than the theoretical predictions for the range of photon energies from 10 to 100 keV. For the range 1 to 10 keV, the experimental data are on average 7% higher than the theoretical predictions.

Fig. 4.2.4.4 is given as a rapid means of comparing theory and experiment. For more detailed information, see Saloman & Hubbell (1986), Saloman *et al.* (1988), and Creagh (1990).

### 4.2.4.4. *Uncertainty in the data tables*

It is not possible to generalize on the accuracy of the experimental data sets. Creagh & Hubbell (1987) have shown that many experiments for which the precision quoted by the author is high differ from other accurate measurements by a considerable amount. It must be stressed that the experimental apparatus has to be chosen so that it is appropriate for the atomic system being investigated. Details concerning the proper choice of measuring system are given in Section 4.2.3. Within about 200 eV of an absorption edge, deviations of up to 200% may be observed between theory and experiment. This is the region in which XAFS and XANES oscillations occur.

With respect to the theoretical data: the detailed agreement between the several methods for calculating the photo-effect cross sections is quite remarkable and it is estimated that the reliability of these data is to within 2% for the energy range considered in this compilation. Some problems may exist, however, close to the absorption edges. Errors in the calculation of the Rayleigh and the Compton scattering cross sections are assessed to be of the order of 5%. Because the greater proportion of total attenuation is photoelectric, the accuracy of the total scattering cross section should be much better than 5% and usually close to 2%.

## 4.2.5. Filters and monochromators (By D. C. Creagh)

### 4.2.5.1. *Introduction*

All sources of X-rays, whether they be produced by conventional sealed tubes, rotating-anode systems, or synchrotron-radiation sources, emit over a broad spectral range. In many cases, this spectral diversity is of concern, and techniques have been developed to minimize the problem. These techniques





references