4.2.3.5. *Comments*

For reliable experiments using XAFS and XANES to be undertaken, intense-radiation sources must be used. Synchrotron-radiation sources are such a source of highly intense X-rays. Their ready availability to experimenters and the comparative simplicity of the equipment required to perform the experiments have made experiments involving XAFS and XANES very much easier to perform than has hitherto been the case.

At some synchrotron-radiation sources, database and program libraries for the storage and analysis of XAFS and XANES data exist. These are usually part of the general computing facilities (Pantos, 1982).

Crystallographers seeking information concerning the nature and extent of these computer facilities can find such information by contacting the computer centre at one of the synchrotron-radiation establishments listed in Table 4.2.3.1.

4.2.4. X-ray absorption (or attenuation) coefficients (By D. C. Creagh and J. H. Hubbell)

4.2.4.1. *Introduction*

This data set is intended to supersede those data sets given in *International Tables for X-ray Crystallography*, Vols. III (Koch, MacGillavry & Milledge, 1962) and IV (Hubbell, McMaster, Del Grande & Mallett, 1974).

It is not intended here to give a detailed bibliography of experimental data that have been obtained in the past 90 years. This has been the subject of a number of publications, *e.g.* Saloman & Hubbell (1987), Hubbell, Gerstenberg & Saloman (1986), Saloman & Hubbell (1986), and Saloman, Hubbell & Scofield (1988). Further commentary on the validity and the quality of the experimental data in existing tabulations has been given by Creagh & Hubbell (1987) and Creagh (1987).

Existing tabulations of X-ray attenuation (or absorption) cross sections fall into three distinct categories: purely theoretical, purely experimental, and an evaluated mixture of theoretical and experimental data.

Compilations of the purely theoretically derived data exist for:

photo-effect absorption cross sections (Storm & Israel, 1970; Cromer & Liberman, 1970; Scofield, 1973; Hubbell, Veigele, Briggs, Brown, Cromer & Howerton, 1975; Band, Kharitonov & Trzhaskovskaya, 1979; Yeh & Lindau, 1985);

Compton scattering cross sections (Hubbell *et al.*, 1975);

Rayleigh scattering cross sections (Hubbell *et al.,* 1975; Hubbell & Øverbø, 1979; Schaupp, Schumacher, Smend, Rullhausen & Hubbell, 1983).

Many purely experimental compilations exist, and the cross-section data given in computer programs used in the analysis of results in X-ray-fluorescence spectroscopy, electron-probe microanalysis, and X-ray diffraction are usually (evaluated) compilations of several of the following compilations: Allen (1935, 1969), Victoreen (1949), Liebhafsky, Pfeiffer, Winslow & Zemany (1960), Koch *et al.* (1962), Heinrich (1966), Theisen & Vollath (1967), Veigele (1973), Leroux & Thinh (1977), Montenegro, Baptista & Duarte (1978), and Plechaty, Cullen & Howerton (1981). If a comparison is made between these data sets, significant discrepancies are found, and questions must be asked concerning the reliability of the data sets that are compared. Jackson & Hawkes (1981) and Gerward (1986) have produced sets of parametric tables to simplify the application of X-ray attenuation data for the solution of problems in computer-aided tomography and X-ray-fluorescence analysis.

Compilations by Henke, Lee, Tanaka, Shimambukuro & Fujikawa (1982) and the earlier tables of McMaster, Del Grande, Mallett & Hubbell (1969/1970) are examples of the judicious application of both theoretical and experimental data to produce a comprehensive data set of X-ray interaction cross sections.

Because of the discrepancies that appear to exist between experimental data sets, the IUCr Commission on Crystallographic Apparatus set up a project to establish which, if any, of the existing methods for measuring X-ray interaction cross sections (X-ray attenuation coefficients) and which theoretical calculations could be considered to be the most reliable. A discussion of some of the major results of this project is given in Section 4.2.3. A more detailed description of this project has been given by Creagh & Hubbell (1987, 1990).

In this section, tabulations of the total X-ray interaction cross sections σ and the mass absorption coefficient μ_m are given for a range of characteristic X-ray wavelengths [Ti $K\alpha$ 2.7440 Å (or 4.509 keV) to Ag $K\beta$ 0.4470 Å (or 24.942 keV)]. The interaction cross sections are expressed in units of barns/atom ($1\ \text{barn} = 10^{-28}\ \text{m}^2$) whilst the mass absorption coefficient is given in $\text{cm}^2\ \text{g}^{-1}$. Table 4.2.4.1 sets out the wavelengths of the characteristic wavelengths used in Tables 4.2.4.2 and 4.2.4.3, which list values of σ and μ_m, respectively.

Users of these tables should be aware of three important facts.

(i) The values given in the tables are derived for the case of isolated atoms, and cooperative effects may become important in condensed phases (Section 4.2.3).

(ii) The values are based solely on theoretical calculations.

(iii) The limits to the reliability of the data when compared with experimental values are shown in Fig. 4.2.4.4.

The linear attenuation coefficient μ_l in units of cm^{-1} can be defined operationally as

$$\mu_l = \left(\ln \frac{I_o}{I}\right) \Big/ t \qquad (4.2.4.1)$$

from the exponential attenuation relationship

$$\frac{I}{I_0} = \exp(-\mu_l t) \qquad (4.2.4.2)$$

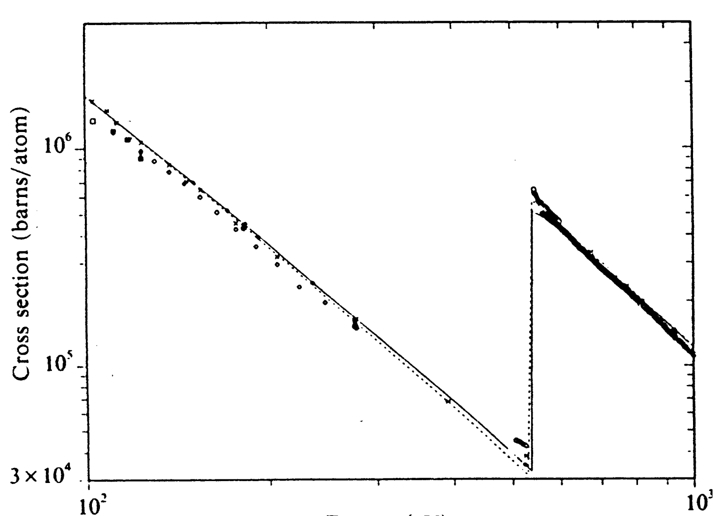

Fig. 4.2.4.1. Agreement between theory and experiment for oxygen ($Z = 8$) in the 'soft' X-ray region. The solid line is for the Scofield (1973) values without renormalization and the dotted line is for the semi-empirical data of Henke *et al.* (1982).

references