

UCRL 50174 SEC 1 TID-4500, UC-34 Physics

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UCRL-50174 Sec. I

Service.

COMPILATION OF X-RAY CROSS SECTIONS SECTION I

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J. H. Hubbell, National Bureau of Standards

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Foreword

Section I of UCRL-50174 describes the methods used in obtaining the compilation of x-ray cross sections. Section II reports the compilation cross sections, Section III gives the supporting data used to create the compilation, and Section IV gives the cross sections at energies useful to crystallographers.

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COMPILATION OF X-RAY CROSS SECTIONS SECTION I

Abstract

X-ray cross sections have been compiled in the range from 1 keV to 1 MeV. To obtain this compilation, existing experimental x-ray total cross section data and theoretical cross section calculations were surveyed. Coherent, incoherent, photoelectric, and total cross sections are given for 87 elements in both barns/atom and cm²/g. Miscellaneous data are also given. The coherent (Rayleigh)

scattering cross section and the incoherent (Compton) scattering cross
sections were computed. The photoelectric cross sections were obtained
by least squares fitting of experimental
data, theory, and interpolation of experiment and theory. Three ranges of uncertainty for the total cross sections are
given, and a list of 84 data sources is
presented.

Introduction

A compilation of x-ray cross sections has been made covering the range of 1 keV to 1 MeV. To obtain this compilation the existing x-ray total cross section data and the theoretical photoelectric cross section calculations were surveyed. This survey was made by combining the existing data files maintained at the Lawrence Radiation Laboratory, Livermore (LRL) by N. Kerr Del Grande and J. H. Mallett with the

J. H. Hubbell file at the National Bureau of Standards.

A preliminary set of cross section tables was published in January 1967 in UCRL-50174, Sec. II. The final compilation was published in July 1969 as UCRL-50174, Sec. II, Rev. 1. The compilation is also available on magnetic tape. The tape facilities are being maintained at LRL by R. J. Howerton and at the DASA Data Center, Santa Barbara, California.

Scattering Cross Sections

The scattering cross sections presented in the compilation were computed using form factors

available in the literature. The formulations used are described below.

COHERENT SCATTERING CRCSS SECTION

The coherent (Rayleigh) scattering cross section was calculated using the expression:

$$\sigma_{\rm coh} = \int \frac{d\sigma_{\rm coh}}{d\Omega} d\Omega = 2\pi \int_0^{\pi} \frac{F^2(\theta, E) r_0^2}{2}$$

$$\times (1 + \cos^2 \theta) \sin \theta \, d\theta$$
 (1)

in which

 $r_0^2 = 7.9398 \times 10^{-2}$ barns, the square of the classical electron radius

θ = 2Φ, the angle between the incident and scattered photon directions where Φ is the Bragg-angle parameter used, e.g., by Stinner, McMaster, and Del Grande¹, Ibers², Cromer and Waber,³ and Brown⁴

 $d\Omega = 2\pi \sin \theta \ d\theta$, the solid angle between cones with angles θ and $\theta + d\theta$

For the atomic form factor $F(\theta, E)$ we used the relativistic Dirac-Slater data of Cromer and Waber³ in the form of their nine-parameter analytical fit to their theoretical results:

$$F(\theta, E) = \sum_{i=1}^{4} A_i \exp(-B_i X^2) + C$$
 (2)

where

$$X = \frac{\sin(\theta/2)}{\lambda} = \frac{E \sin(\theta/2)}{12.39831}$$

with λ in Angstroms and E in keV. The coefficients A_i , B_i , and C are given for

elements Z = 1 to 102 and a number of ions. These data are valid only for the range $0 \le X \le 2$, so a semilogarithmic extrapolation was made in order to integrate Eq. (1) to backward angles for photon energies above 25 keV.

INCOHERENT SCATTERING CROSS SECTION

The incoherent (Compton) scattering cross section was calculated using the expression

$$\sigma_{\rm inc} = \int \frac{{\rm d}\sigma_{\rm inc}}{{\rm d}\Omega} \ {\rm d}\Omega = 2\pi \int_0^\pi \ ZS(\theta, E)$$

$$\times \left(\frac{d\sigma}{d\Omega}\right)_{KN} \sin\theta \,d\theta$$
, (3)

in which

Z = atomic number

 $S(\theta, E)$ = incoherent scattering form factor

$$\left(\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}\right)_{\mathrm{KN}} = \frac{\mathbf{r}_0^2}{2} \left[1 + k(1 - \cos\theta)\right]^{-2}$$

$$\times \left[1 + \cos^2\theta + \frac{k^2(1 - \cos\theta)^2}{1 + k(1 - \cos\theta)}\right].$$

The $\left(\frac{d\sigma}{d\Omega}\right)_{\rm KN}$ is the usual Klein-Nishina formula where k = E/mc² = E/511 (E is in keV), and r_0 and θ are defined as in Eq. (1).

The values used for $S(\theta, E)$ were taken from the calculations of Cromer and Mann⁵ for 35 elements. These elements are listed in Table I. The cross section values for the remaining elements were obtained from a sliding polynomial fit as

Table I. Elements for which Hartree-Fock form factors are available.

Z	Element	Z	Element	Z	Element
2	Helium	25	Manganese	51	Antimony
3	Lithiura	29	Copper	54	Xenon
4	Beryllium	30	Zinc	55	Cesium
7	Nitrogen	33	Arsenic	56	Barium
10	Neon	36	Krypton	63	Europium
11	Sodium	37	Rubidium	70	Ytterbium
12	Magnesium	38	Strontium	75	Rhenium
15	Phosphorus	42	Molybdenum	79	Gold
18	Argon	43	Technetium	80	Mercury
19	Potassium	46	Palladium	83	Bismuth
20	Calcium	47	Silver	86	Radon
24	Chromium	48	Cadmium		

shown in Figs. 1 through 25 of Sec. III. At low energies the curves are far from smooth, and we cannot assign an accuracy to the interpolation.

Additional information and references on S(0, E) and incoherent scattering are given, e.g., by Pirenne, ⁶ Grodstein (see especially the appendix, p. 51 through 53), ⁷ Evans, ⁸ Brown, ⁹ and Veigele, Tracy, and Henry, ¹⁰

Other corrections to the Klein-Nishina formula <u>not</u> considered here are:

- 1. Effects of atomic electron velocity (target electron not initially at rest)
- 2. Radiative and double-Compton (two outgoing photons) corrections

The first of these two corrections may be significant in the region considered here but it is too poorly known experimentally or theoretically (see, e.g., Motz and

Missoni, 11 and DiLazzaro and Missoni 12) to apply to the present compilation. The second correction is negligible below 1 MeV (~ 0.25% at 4 MeV—see, e.g., Mork, 13 and Hubbell and Berger 14).

SCATTERING CROSS SECTIONS FOR HYDROGEN

The coherent and incoherent form factors of hydrogen were calculated from the exact expressions 6:

$$F(\theta, E) = (1 + 4\pi^2 a_0^2 X^2)^{-1}$$

and

$$S(\theta, E) = 1 - F^{2}(\theta, E)$$
 (4)

where

 $a_0 = 0.529167$, the Bohr radius in angstroms.

Photoelectric Cross Sections

CROSS SECTION VALUES

The photoelectric cross sections were obtained using a combination of methods. The following paragraphs describe the methods used to obtain the values for the final fit for each element:

- 1. Whenever sufficient experimental total cross section data were available, the compilation values were obtained by subtracting the calculated scattering cross sections from the data points. No experimental points were used for the fit in the region where scattering is greater than 95% of the total. These data points, however, were used to check the accuracy of the total cross section.
- 2. The theoretical calculations of Schmickley and Pratt¹⁵ were used for the following 14 elements for energies above 10 keV: Z = 13, 20, 26, 29, 42, 47, 50, 60, 74, 78, 79, 82, 84, and 92.
- 3. A third-order log-log least squares fit to the theoretical values of Schmickley and Pratt¹⁵ was made across Z to obtain cross section values for those elements not calculated by Schmickley and Pratt.
- 4. Two types of further third-order log-log least squares fits were made
 (a) using all elements in the compilation, and (b) using only those elements for which the best experimental data exist.

Additional data and literature references on the atomic photoeffect are given, e.g., by Davisson, ¹⁶ Hultberg, Nagel, and Olsson, ¹⁷ Rakavy and Ron, ¹⁸ and Hall and Sullivan. ¹⁹

K-EDGE PHOTOEFFECT

The use of the K-edge has many applications in x-ray experiments. An effort

has been made to present as consistent a set of values as possible for these particular cross sections. The edge energies used are those of Hagström, et al. 20

The energies for the fluorescence x-ray are those given by Fine and Hendee. 21

The K-edge characteristics are illustrated in Figs. 26 through 28 of Sec. III. Figure 26 shows the photoelectric jump ratios for those elements in the compilation with $Z \ge 11$ (K-edge energy ≥ 1 keV). Figures 27 and 28 show the upper and lower values of the photoelectric cross section at the edge.

The jump ratio values, J, were fit to the second order by the equation:

$$\ln J = \sum_{i=0}^{2} C_{i} (\ln Z)^{i}, \qquad (5)$$

and the cross section values were fit to the first order by the equation:

$$\ln \sigma = \sum_{i=0}^{1} C_i (\ln Z)^i, \qquad (6)$$

where σ is in barns/atom. The fit coefficients for these equations are given in Table II.

Since recent experiments 22,23,24 have shown resonance structure in the vicinity of the K-edge (suggesting that the concept of a jump ratio is only an approximation), it is not surprising to find deviations from the fit values.

Table II. K-Edge fit coefficients.

i	Jump ratios	σ(upper)	σ(lower)
0	3.14115	18.1397	14.6118
1	-0.214745	-2.33148	-1.89418
2	-0.0311536		

Data Processing

GENERAL

Published and unpublished experimental data have been used to establish the present compilation. The description of each experiment has been reviewed in an attempt to evaluate the results. Some of the points considered in the evaluation include:

- (1) Inadequate correction for sample impurities
- (2) Small angle scattering detection due to poor collimation
- (3) Lack of monoenergetic sources of x-rays
- (4) Obvious typographical errors
- (5) Unexplainable systematic errors
 All data points disagreeing more than
 10% with the fit through values of several
 data sources were arbitrarily removed
 from the data file. The final data file

used consists of approximately 10,000 cross section values for 87 elements from 84 data sources.

DATA SOURCES

The data sources used are listed in Appendix A, and have been assigned numbers from 1 through 91. Also given are unnumbered supplemental data references of a similar nature which the reader may find useful. In making the least squares fits, the data from each data source were weighted according to the accuracy as indicated by the experimenter. These weighting factors are listed in Table III.

For some elements experimental data below 1 keV were used in obtaining the fits. These elements are listed in Table IV. Elements for which no experimental data

Table III. Weights greater than one assigned to experimental sources.

Source	Weight	Source	Weight	Source	Weight
3	3	28	5	63	2
5	2	29	3	65	2
7	3	30	2	66	3
8	4	31	2	67	3
9	3	33	2	69	2
11	10	34	2	70	2
12	2	37	2	73	3
13	2	39	5	76	2
16	3	40	5	77	2
17	2	42	3	78	3
19	2	45	2	81	2
20	2	46	3	82	3
23	2	47	5	83	3
24	2	48	3	87	2
25	2	55	2		
26	5	62	2		

Table IV. Elements with experimental data below 1 keV in file.

9 F	17 Cl
10 Ne	18 Ar
12 Mg	36 Kr
13 Al	47 Ag
16 S	
	10 Ne 12 Mg 13 Al

were available are listed in Table V. A complete listing of all elements and their corresponding data sources is given in Fig. 1.

INTERPOLATED DATA

To fill out the data bank, interpolated values of the photoelectric cross section were used as described under "Photoelectric Cross Sections." These appear as the following three references in the data source list:

Reference 10

This interpolation was made using a selected number of elements for which the best experimental data exist. The sources used provided extensive coverage with quoted accuracies of better than 2%.

Reference 89

This interpolation was made using the theoretical photoelectric cross sections of Schmickley and Pratt. 15

Reference 90

This interpolation was made in an iterative manner using all data in the compilation to force a smooth fit across Z at a given energy and also across energy at a given Z. The final cross Z

Table V. Elements with no experimental data in file.

14 Si	43 Tc	66 Dy
15 P	44 Ru	68 Er
19 K	55 Cs	71 Lu
1 31 Ga	59 Pr	75 Re
37 Rb	61 Pm	76 Os
39 Y	63 Eu	86 Rn

fits used in this interpolation are shown in barns/atom in Figs. 29 through 81 of Sec. III.

The interpolation was made first across Z at the compilation grid energies and cross sections. These interpolated values were then inserted in each element's data file, and the fits were made for each shell to obtain the interim compilation values. The process was repeated again and again until a consistent set of fits was obtained,

DATA FITTING

The data points for each element were fitted by a polynomial on a log-log scale for each shell. The fit parameters so derived for each element are given in Sec. II. The fit was made to the photo-electric cross section which was obtained by subtracting the calculated scattering cross sections from the total cross sections in the data file. No fits were made inside the L and M edges. The cross sections in these regions were obtained by using jump ratios calculated from the theoretical values of Rakavy and Ron. 18

Data tabulations for those elements with experimental values are given in Sec. III.

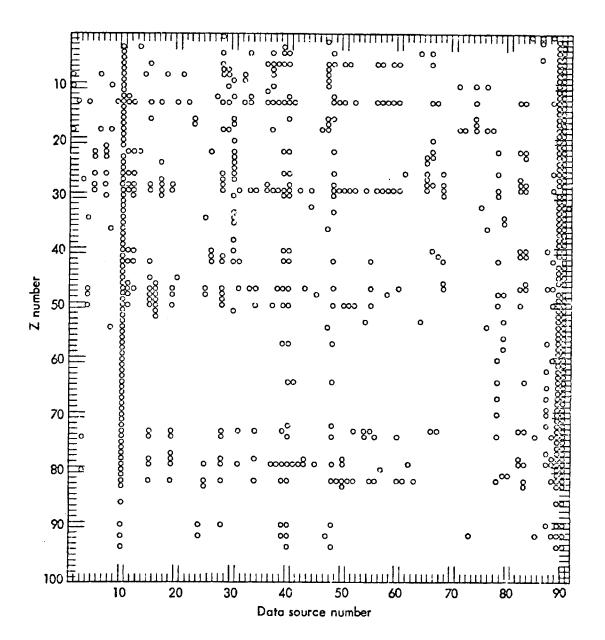


Fig. 1. Data sources of compilation of x-ray cross sections.

Uncertainty of Compilation Values

The authors have estimated the ranges of uncertainties in values of the total cross section. These ranges of uncertainties fall predominately into three categories:

- $A. < \pm 2\%$
- B. ± 2 to 5%
- C. ± 5 to 15%

CATEGORY A (< ±2%)

This category applies (except just above edges as noted in Category C) over the energy region 6 to 40 keV for several elements. In the authors' opinion, there is an adequate number of independent experimental data sources, with sufficient overlap and consistency to assign a ±2%

envelope of uncertainty for these elements in this energy range.

The authors also include in Category A the region for all elements where incoherent scattering comprises more than 90% of the total cross section.

CATEGORY B (± 2 to 5%)

Except for the elements singled out for Category C, Category B applies to the energy region 2 to 6 keV for all elements, 6 to 40 keV for elements not in Category A,

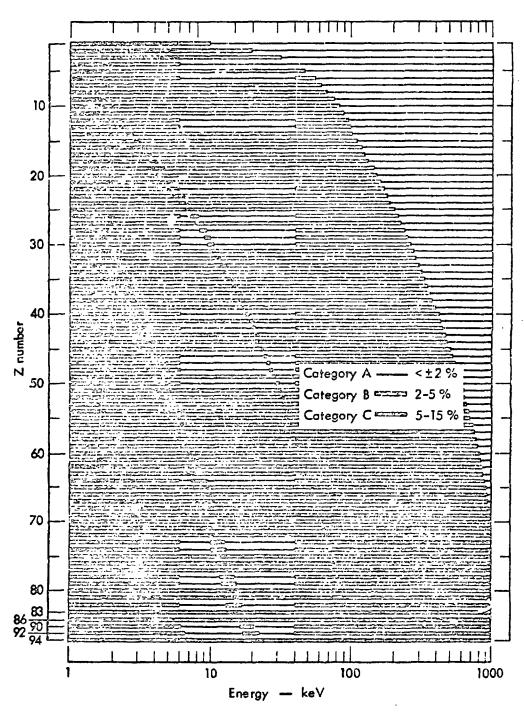


Fig. 2. Estimated ranges of uncertainties in values of the total cross sections.

and above 40 keV except for the scattering-dominated region specified in Category A.

For energies above 2 keV, it was noted that available experimental data could be represented by least-squares third-order log-log fits across Z. 'The degree of consistency of the individual data points for well-measured elements with these fits formed a partial basis for the ± 2 to 5% uncertainty assigned to Category B data.

CATEGORY C (± 5 to 15%)

The largest uncertainties are applicable to compilation values in the region of the K, L, M, and N absorption edges, where resonance-type structure can occur but is ignored in this compilation. This region includes the energy region between edges and extends in some instances as much as 1 keV above the edge in question (see, e.g., Lytle, Del Grands and Oliver, and Boster and Edwards for examples of K-edge fine structure).

The authors also include in Category C the extrapolated values in:

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- The energy region below 8 keV of elements hydrogen, helium, and lithium
- 2. The energy region 1 to 2 keV for all elements
- The energy region from the K-edge energy to 5% above the K-edge energy (especially for higher Z elements)

Although experimental uncertainties in some of these cases greatly exceed 15%, the total cross sections here are considered known theoretically to within this uncertainty.

Direct comparisons of this compilation with other independent compilations and recently published and unpublished experimental work substantiate the accuracy quoted. In fact, many of the quoted uncertainties may be somewhat conservative.

Figure 2 is a graphical representation of the ranges of uncertainty. Given are the three levels of uncertainty for each element as a function of energy.

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