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EMPIRICAL REPRESENTATION OF
PHOTOELECTRIC CROSS SECTIONS

by

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ABSTRACT

The problem of providing empirical fits to tabulated photoelectric cross sections is discussed, and two formulas which may be used for this purpose are recommended. These formulas are:

$$\sigma_1(E_\gamma) = \sum_{k=1}^{n_1} a_k E_\gamma^{1-k}$$

and

$$\sigma_2(E_\gamma) = \exp \left[\sum_{k=1}^{n_2} b_k (\ln E_\gamma)^{k-1} \right].$$

Nuclear researchers frequently have need of photon cross-section information in processing nuclear data. An example is the study of $(n,n'\gamma)$ reactions, where it is necessary to correct for gamma-ray attenuation in the scattering samples before gamma-ray production cross sections can be computed from the raw gamma-ray yield data. Compilations of photon cross sections are available, and these are periodically updated by specialists in the field (e.g., see Refs. 1 and 2).

Users of cross-section compilations must interpolate to determine cross sections at energies not listed in these compilations. Since photon cross sections vary smoothly with energy (except near absorption edges), it is reasonable to try to represent them by analytic formulas and thereby reduce the number of parameters required for calculations.³ In applications, one is generally not concerned with justification of the formula used to calculate cross-section values, so it is appropriate to consider any analytic functions that provide a good representation of the energy dependence of the cross section in question.

The subject of this report is the representation of photoelectric cross sections. Three empirical formulas that have been used for this purpose are

$$\sigma_1(E_Y) = \sum_{k=1}^{n_1} a_k E_Y^{1-k}, \quad (\text{e.g., see Ref. 3}) \quad (1)$$

$$\sigma_2(E_Y) = \exp \left[\sum_{k=1}^{n_2} b_k (\ln E_Y)^{k-1} \right], \quad (\text{e.g., see Ref. 2}) \quad (2)$$

and

$$\sigma_3(E_Y) = \exp \left[c_1 + \left(\sum_{k=2}^{n_3} c_k E_Y^{k-2} \right) \ln E_Y \right], \quad (\text{e.g., see Ref. 4}) \quad (3)$$

where $\{a_k\}$, $\{b_k\}$, and $\{c_k\}$ are sets of adjustable parameters. Each of these formulas has been demonstrated to be satisfactory for representation of photoelectric cross-section data over limited ranges of photon energy.²⁻⁴

The objective of the present study was to determine which of these formulas yields the best results. It is well known that photoelectric cross sections are discontinuous at absorption edges, but not so well known that these discontinuities are not sharp "sawtooths" but somewhat rounded.⁵ The present discussion overlooks this consideration and assumes the "sawtooth" model. The error is probably not too large, except in the vicinity of the absorption edges. Equations 1-3 were fitted by least-squares analysis⁶ to the total photoelectric cross sections ($Z = 1$ to $Z = 100$, E_Y above the K edge) from the Storm and Israel compilation.¹ The energy ranges involved in the fitting calculations are indicated in Table I. The

TABLE I. Summary of the Largest Deviations Observed for Empirical Fits to the Storm and Israel Total Photoelectric Cross-section Compilation¹

Z	E_Y Range, ^a MeV	Equation 1		Equation 2		Equation 3	
		No. of Parameters	Maximum Deviation, %	No. of Parameters	Maximum Deviation, %	No. of Parameters	Maximum Deviation, %
1	0.001-0.015	6	0.1	4	1.0	7	0.2
2	0.001-0.04	6	0.4	4	2.4	8	1.5
3	0.001-0.08	7	1.1	4	3.0	7	2.4
4	0.001-0.1	7	0.8	4	2.5	9	2.0
5	0.001-0.15	8	2.4	4	2.1	9	2.3
6	0.001-0.2	8	1.8	4	2.8	8	4.2
7	0.001-0.3	8	1.6	4	4.3	9	4.3
8	0.001-0.4	9	1.1	4	4.4	9	5.2
9	0.001-0.4	9	1.4	4	4.4	9	5.5
10	0.001-0.4	10	2.8	4	5.9	9	9.9
11	0.001073-0.6	10	4.0	6	2.9	9	9.2
12	0.001305-0.8	10	3.1	6	1.9	9	7.1
13	0.00156-1.0	11	2.8	6	2.1	9	8.1
14	0.001839-1.0	11	2.9	6	1.9	9	5.5
15	0.002144-1.5	11	2.1	8	1.7	9	6.4
16	0.002472-1.5	11	1.5	8	1.2	9	6.8
17	0.002824-2.0	11	1.8	8	1.2	9	4.7
18	0.003209-2.0	11	1.4	8	1.0	9	6.7
19	0.003607-3.0	11	2.3	7	1.7	9	6.8
20	0.004097-4.0	11	2.0	7	2.0	9	6.4
21	0.004491-5.0	11	1.7	9	1.3	9	1.4
22	0.004866-6.0	11	1.4	7	2.0	9	7.5
23	0.005465-6.0	11	1.4	7	2.2	9	8.1
24	0.005989-8.0	10	1.5	7	1.8	9	9.4

TABLE 1 (Contd.)

Z	E _γ Range, ^a MeV	Equation 1		Equation 2		Equation 3	
		No. of Parameters	Maximum Deviation, %	No. of Parameters	Maximum Deviation, %	No. of Parameters	Maximum Deviation, %
25	0.006539-8.0	10	1.2	9	0.8	9	10.5
26	0.007112-30.0	10	1.3	6	2.1	9	11.2
27	0.007709-30.0	10	1.7	6	2.8	9	2.4
28	0.008332-15.0	10	1.4	9	1.7	9	13.2
29	0.008981-15.0	10	1.0	8	2.3	9	12.6
30	0.009659-20.0	9	2.1	7	4.0	9	11.8
31	0.01037-20.0	9	2.4	7	3.5	9	19.0
32	0.0111-20.0	9	2.4	9	2.8	9	16.9
33	0.01187-30.0	9	2.7	7	2.8	7	20.2
34	0.01266-30.0	9	2.6	7	2.4	7	18.2
35	0.01347-30.0	9	2.4	7	2.7	7	17.0
36	0.01432-40.0	9	2.9	7	2.4	8	15.4
37	0.0152-40.0	9	2.0	7	2.1	8	18.7
38	0.01611-50.0	9	1.8	7	2.5	8	16.9
39	0.01704-60.0	9	1.9	7	3.4	9	14.8
40	0.018-60.0	9	2.0	7	3.0	9	12.9
41	0.01899-60.0	9	1.8	7	2.9	9	11.6
42	0.02-80.0	8	2.8	7	3.9	9	11.4
43	0.02104-80.0	8	2.1	7	3.3	9	10.9
44	0.02212-100.0	8	3.2	7	4.9	9	13.5
45	0.02322-100.0	8	1.7	7	3.0	9	11.6
46	0.02435-100.0	8	1.8	7	3.0	9	11.0
47	0.02551-100.0	8	2.8	7	3.0	9	10.9
48	0.02671-100.0	8	1.6	7	2.8	9	11.3
49	0.02794-100.0	8	1.4	7	2.7	9	10.7
50	0.0292-100.0	8	2.8	8	2.3	9	11.1
51	0.03049-100.0	8	1.5	8	2.8	9	10.3
52	0.03181-100.0	8	1.3	7	2.6	9	10.6
53	0.03317-100.0	8	1.2	9	1.1	9	11.1
54	0.03456-100.0	8	1.4	9	2.1	9	10.2
55	0.03599-100.0	9	1.4	7	2.6	8	15.9
56	0.03744-100.0	8	1.3	7	2.4	9	10.3
57	0.03893-100.0	9	1.4	10	1.4	8	14.7
58	0.04044-100.0	8	1.7	7	2.5	9	10.3
59	0.04199-100.0	8	1.5	9	2.2	9	10.1
60	0.04357-100.0	9	1.4	9	1.4	9	9.9
61	0.04518-100.0	9	1.5	7	2.7	9	10.2
62	0.04683-100.0	8	1.6	6	2.9	9	9.9
63	0.04852-100.0	8	1.4	7	1.9	9	8.5
64	0.05024-100.0	8	1.4	6	2.2	9	10.0
65	0.052-100.0	8	1.3	6	2.1	9	9.8
66	0.05379-100.0	8	1.4	6	2.2	9	9.6
67	0.05542-100.0	8	1.3	6	1.9	9	9.6
68	0.05709-100.0	8	1.2	6	1.8	9	9.7
69	0.05879-100.0	8	1.2	6	1.8	9	9.4
70	0.06113-100.0	8	1.2	6	1.5	9	9.3
71	0.06332-100.0	8	1.2	6	1.4	9	9.1
72	0.06535-100.0	8	1.4	6	1.5	9	9.4
73	0.06742-100.0	8	1.2	6	1.4	9	8.2
74	0.06953-100.0	8	1.4	6	1.9	9	8.0
75	0.07168-100.0	8	1.4	6	2.0	9	8.6
76	0.07387-100.0	7	1.4	8	1.8	9	8.4
77	0.07611-100.0	7	1.8	7	1.8	9	8.3
78	0.0784-100.0	7	1.8	7	2.8	9	7.8
79	0.08073-100.0	7	1.7	8	1.4	9	7.4
80	0.0831-100.0	7	1.7	7	1.5	9	7.6
81	0.0853-100.0	7	1.5	7	1.3	9	7.6
82	0.088-100.0	7	1.7	6	2.4	9	7.0
83	0.09053-100.0	6	1.8	6	2.3	9	7.3
84	0.09311-100.0	6	1.4	8	1.4	9	6.8
85	0.09573-100.0	6	1.5	8	1.4	9	7.3
86	0.0984-100.0	6	1.6	8	2.2	9	7.2
87	0.1011-100.0	6	1.8	6	1.8	9	6.6
88	0.1039-100.0	6	1.5	8	1.9	9	7.0
89	0.1068-100.0	6	1.6	6	2.1	9	6.5
90	0.1097-100.0	6	1.5	6	1.9	9	6.5
91	0.1126-100.0	6	1.5	7	1.8	9	6.4
92	0.1156-100.0	6	1.5	6	1.7	9	5.7
93	0.1187-100.0	6	1.9	6	1.7	9	6.1
94	0.1218-100.0	6	1.9	6	1.7	9	6.0
95	0.125-100.0	6	1.8	6	1.8	9	5.9
96	0.1283-100.0	6	1.6	6	1.9	9	6.2
97	0.1316-100.0	6	1.7	6	1.9	9	6.2
98	0.135-100.0	7	1.8	6	2.0	9	6.5
99	0.1385-100.0	7	1.6	6	2.4	9	6.7
100	0.1421-100.0	8	1.9	6	2.4	9	6.1

^aLow end of energy range is either 0.001 MeV or the K-edge energy (whichever is larger).
Maximum deviations exceeding 3% are underlined.

quality of the fits were compared by means of the residual, R , where

$$R = \sum_{i=1}^N \left(\frac{\sigma_{Ti} - \sigma_{Ei}}{\sigma_{Ei}} \right)^2, \quad (4)$$

N is the number of tabulated energies, σ_{Ti} is the calculated empirical cross section for the i th energy, and σ_{Ei} is the corresponding tabulated cross section. Since Eq. 1 is linear in the parameters $\{a_k\}$, the normal equations required by the least-squares method can be derived directly from Eq. 4. Equations 2 and 3 are nonlinear in their respective parameters $\{b_k\}$ and $\{c_k\}$, but their logarithms are linear. This suggests derivation of the normal equations from the expression

$$S = \sum_{i=1}^N (\ln \sigma_{Ti} - \ln \sigma_{Ei})^2. \quad (5)$$

It is easy to prove the limit relation

$$S \rightarrow R \text{ as } \{\sigma_{Ti} \rightarrow \sigma_{Ei}\},$$

so minimization of S is essentially equivalent to minimization of R .

The normal equations were solved by Gauss-Jordan reduction with all computations performed on a digital computer. The analysis for each element (value of Z) proceeded as follows: The best two-parameter fit was determined for each formula, and values of the residuals R were computed from Eq. 4. The number of adjustable parameters used was then increased, and a new set of residuals R was computed. This procedure was repeated either until no significant improvement in the fit was observed by addition of more adjustable parameters, or until limitations were encountered in the arithmetic capacity of the computer. The percentage differences between the tabulated cross section and the empirical cross sections were also calculated by the computer at each energy.

The results of this fitting study are summarized in Figs. 1-4 and in Table I. The residuals R defined by Eq. 4 are plotted in Figs. 1-4 against the number of arbitrary parameters used in the least-squares fittings. The solid squares correspond to fits made with Eq. 1, the crosses correspond to fits made with Eq. 2, and the open circles correspond to fits made with Eq. 3. The accuracy claimed for the total photoelectric cross sections tabulated by Storm and Israel is 1-6 keV, 10%; 6-200 keV, 3%; and >200 keV, 10%. Agreement between the tabulated and calculated cross sections within $\pm 3\%$ at all the tabulated energies has been considered in the present work as indication of a "perfect fit." Table I lists the maximum absolute percentage deviations between the calculated and tabulated cross sections which

Fig. 1. Residuals R for Empirical Fits to Total Photoelectric Cross Sections vs Number of Adjustable Parameters: $Z = 1 \rightarrow Z = 25$ (see text). ANL Neg. No. 116-1000.

Fig. 2. Residuals R for Empirical Fits to Total Photoelectric Cross Sections vs Number of Adjustable Parameters: $Z = 26 \rightarrow Z = 50$ (see text). ANL Neg. No. 116-1003.

Fig. 3. Residuals R for Empirical Fits to Total Photoelectric Cross Sections vs Number of Adjustable Parameters: $Z = 51 \rightarrow Z = 75$ (see text). ANL Neg. No. 116-1001.

$$\sum_{i=1}^N \left[\frac{\partial^2}{\partial^2} \right]$$

Fig. 4. Residuals R for Empirical Fits to Total Photoelectric Cross Sections vs Number of Adjustable Parameters; $Z = 76 \rightarrow Z = 100$ (see text), ANL Neg. No. 116-1002.

were obtained for least-squares fittings with the indicated formulas and numbers of adjustable parameters. The numbers of adjustable parameters appearing in this table correspond to the maximum values plotted in Figs. 1-4.

Several conclusions can be drawn from an inspection of Figs. 1-4 and Table I. Equation 3 is clearly inferior to the other two formulas for representation of total photoelectric cross sections. For most elements, this formula could not be fitted to the tabulated cross sections to within the $\pm 3\%$ tolerance which was sought. Equations 1 and 2 each seem capable of yielding fits of the desired caliber for most of the elements. Equation 2 provides somewhat better fits for $Z < 30$, Eq. 1 is superior for $Z > 40$. One advantage in the use of Eq. 1 is its functional simplicity. Calculations with Eq. 2 consume more computer time and are probably less accurate because the computer has to evaluate many logarithms.

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REFERENCES

1. E. Storm and H. I. Israel, Photon Cross Sections from 1 keV to 100 MeV for Elements $Z = 1$ to $Z = 100$, Nuclear Data Tables A7, 565 (1970).
2. W. H. McMaster, N. Kerr Del Grande, J. H. Mallet, and J. H. Hubbell, Compilation of X-Ray Cross Sections, UCRL-50174, Secs. I-IV (1969-70).
3. F. Biggs and R. Lighthill, Analytical Approximations for X-Ray Cross Sections, SC-RR-66-452 (1967).
4. D. L. Smith, Empirical Formula for Interpolation of Tabulated Photon Photoelectric Cross Sections, ANL-7796 (Mar 1971).
5. J. H. Hubbell, National Bureau of Standards, Washington, D.C., 20234 (private communication).
6. Yu. V. Linnik, Method of Least Squares and Principles of the Theory of Observations, Pergamon Press, London (1961).