RESOLUTION OF BREMSSTRAHLUNG EXPERIMENTS

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Summary

This paper investigates how mathematical approximations and statistical errors are transmitted into computed cross sections in the analysis of experimental bremsstrahlung yield data. The resolution of bremsstrahlung experiments is defined in analogy with optical resolution and an expression for the practical evaluation of resolution is derived. Methods of cross-section computation, and smoothing and curve-fitting are discussed.

I. ERROR INHERENT IN THE YIELD ANALYSIS

The bremsstrahlung experiment measures the yield of a photonuclear reaction. The corresponding cross section is derived by a transformation calculation. This investigation is concerned with how approximations in the transformation calculation and standard errors of the original discrete set of experimental yield ordinates are propagated into the computed cross section, and how well the computed cross section portrays the true (exact) cross section. It is assumed that the bremsstrahlung spectrum is known and that experimental yield ordinates contain no other than truly statistical errors.

Yield $y(E_{0k})$ and cross section $s(E)$ are related through the normalized bremsstrahlung distribution function $P(E,E_{0k})$ by the integral equation

$$y(E_{0k})=\int_{E_{th}}^{E_{0k}} P(E,E_{0k})s(E)\mathrm{d}E. \tag{1}$$

E_{0k} is the maximum energy of the spectrum, $E=h\nu$ the energy of a photon interacting with a nucleus, and E_{th} the reaction threshold.

Experimental yield data are invariably given as a discrete set of yield values only and not as a continuous function. Thus the knowledge about the yield function is restricted to that of a finite number of yield ordinates, and nothing is known *a priori* about the behaviour of the function between these ordinates. If $y(E_{01})$, $y(E_{02})$, . . ., $y(E_{0k})$, . . ., $y(E_{0p})$ are the yield values corresponding to energies E_{01}, E_{02}, . . ., E_{0k}, . . ., E_{0p}, then the equation

$$y(E_{0k})=\sum_{i=1}^{k} P(E_i,E_{0k})\bar{s}(E_i)\Delta E_i\,;\quad k=1,\ 2,\ .\ .\ .,\ p, \tag{2}$$

must be substituted as an optimum approximation for (1). Here $\Delta E_i=E_{0i}-E_{0,i-1}$,

$$E_i=E_{0i}-\tfrac{1}{2}\Delta E_i,\ \text{and}\ \bar{s}(E_i)\,;\quad i=1,\ 2,\ .\ .\ .,\ p$$

represents a discrete set of cross-section ordinates which are to approximate ordinates $s(E_i)$ of the exact cross section $s(E)$. Any approximation other than

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(2) would make assumptions about $y(E_{0k})$ and $s(E)$, i.e. about the " smoothness " of $y(E_{0k})$, which are not contained in the experimental data.

(2) represents a system of p linear equations in the p unknowns $\bar{s}(E_i)$; $i=1, 2, \ldots, p$, and thus in general has a unique solution and any exact method to solve (2) will give the same unique solution. Existing methods are the total spectrum method (Johns *et al.* 1950), the photon difference method (Katz and Cameron 1951), and the modified total spectrum method of Penfold and Leiss (1958). An iteration method is used by Carver and Lokan (1957).

It is convenient to choose a constant energy interval

$$\Delta E_i=\Delta E_A,$$

and write (2) in matrix form, namely,

$$\mathbf{y}_0=\Delta E_A\mathbf{P}\cdot\bar{\mathbf{s}}. \tag{3}$$

Here

$$\mathbf{y}_0=\begin{bmatrix} y_{01} \\ y_{02} \\ \cdot \\ \cdot \\ y_{0,p-1} \\ y_{0,p} \end{bmatrix};\quad \mathbf{P}=\begin{bmatrix} P_{1,1} & 0 & 0 & \cdot & 0 & 0 \\ P_{2,1} & P_{2,2} & 0 & \cdot & 0 & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 0 & 0 \\ P_{p-1,1} & P_{p-1,2} & \cdot & \cdot & P_{p-1,p-1} & 0 \\ P_{p,1} & P_{p,2} & \cdot & \cdot & P_{p,p-1} & P_{p,p} \end{bmatrix};\quad \bar{\mathbf{s}}=\begin{bmatrix} \bar{s}_1 \\ \bar{s}_2 \\ \cdot \\ \cdot \\ \bar{s}_{p-1} \\ \bar{s}_p \end{bmatrix}$$

and the following abbreviations are used

$$y(E_{0k})=y_{0k},\quad P(E_i,E_{0k})=P_{k,i},\quad \bar{s}_i=\bar{s}(E_i).$$

Defining

$$\mathbf{P}^{-1}=\mathbf{C}=\begin{bmatrix} C_{1,1} & 0 & 0 & \cdot & 0 & 0 \\ C_{2,1} & C_{2,2} & 0 & \cdot & 0 & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 0 & 0 \\ C_{p-1,1} & C_{p-1,2} & \cdot & \cdot & C_{p-1,p-1} & 0 \\ C_{p,1} & C_{p,2} & \cdot & \cdot & C_{p,p-1} & C_{p,p} \end{bmatrix}, \tag{4}$$

solve (3) for $\bar{\mathbf{s}}$, by premultiplying each side of (3) by $(1/\Delta E_A)\mathbf{C}$.
Thus,

$$\bar{\mathbf{s}}=(1/\Delta E_A)\mathbf{C}\cdot\mathbf{y}_0, \tag{5}$$

which is equivalent to the p equations

$$\bar{\mathbf{s}}(E_i)=\frac{1}{\Delta E_A}\sum_{n=1}^{i} C_{i,n}y_{0n};\quad i=1, 2, \ldots, p. \tag{6}$$

From (6) each ordinate $\bar{s}(E_i)$ can be evaluated directly, independently of other ordinates $\bar{s}(E_j)$, $j\neq i$. The coefficients $C_{i,n}$ are related to the coefficients $B_{i,n}$ of Penfold and Leiss (1958) by

$$C_{i,n}=E_iB_{i,n}. \tag{7}$$

Values of $B_{i,n}$ for several values of ΔE_A and for E_{0p} up to 1 BeV are tabulated by Penfold and Leiss (1958) for an integrated-over-angles Schiff spectrum (Schiff 1951).

If $y(E_{0k})$ is given as a continuous function and ΔE_A is chosen smaller than E_{th}, the summation (2) may be started at any energy value E_{00} between 0 and ΔE_A ($E_{00}=E_{01}-\Delta E_A$). Each corresponding set of ordinates $y(E_{0k})$ will define a set of ordinates $\bar{s}(E_i)$, and all the sets $y(E_{0k})$ will define a continuous function $\bar{s}(E)$, where $\bar{s}(E)$ approximates $s(E)$. Any discrete set $\bar{s}(E_i)$, $i=1, 2, 3, \ldots, p$ will lie on $\bar{s}(E)$ rather than on $s(E)$.

The difference $s(E)-\bar{s}(E)$, which is the error introduced by replacing the integration in (1) by the summation of finite difference of (2), will now be computed. It is assumed that $P(E,E_{0k})s(E)$ may be expanded by its Taylor series in any energy interval ΔE_A.

Using the notation

$$\frac{\partial}{\partial E}[P(E,E_{0k})s(E)]_{E=E_i}=[P_{k,i}s_i]',$$

and similarly for higher derivatives, the Taylor expansion of $[P(E,E_{0k})s(E)]$ for the energy interval

$$E_{0,i-1}<E<E_{0i}$$

becomes

$$P(E,E_{0k})s(E)=P_{k,i}s_i+\frac{1}{1!}[P_{k,i}s_i]'(E-E_i)+\frac{1}{2!}[P_{k,i}s_i]''(E-E_i)^2+\ldots \quad (8)$$

With (8) the p yield ordinates y_{0k}; $k=1, 2, \ldots, p$, may be expressed through the p equations

$$y_{0k}=\sum_{i=1}^{k}\left[\int_{E_i-\frac{1}{2}\Delta E_A}^{E_i+\frac{1}{2}\Delta E_A}\{[P_{k,i}s_i]+[P_{k,i}s_i]'(E-E_i)+\tfrac{1}{2}[P_{k,i}s_i]''(E-E_i)^2+\ldots\}\mathrm{d}E\right]; \quad k=1, 2, \ldots, p. \quad (9)$$

Performing the integration, one obtains

$$y_{0k}=\sum_{i=1}^{k}\left\{[P_{k,i}s_i]\Delta E_A+[P_{k,i}s_i]''\frac{\Delta E_A^3}{24}+[P_{k,i}s_i]^{(N)}\frac{\Delta E_A^5}{1920}+\ldots\right\}; \quad k=1, 2, \ldots, p,$$

where the nth term in the bracket is of order

$$\Delta E_A^{2n-1}/(2n-1)!\,2^{2n-2},$$

i.e. the series are strongly convergent, and a sufficiently good approximation is

$$y_{0k}\simeq\sum_{i=1}^{k}P_{k,i}s_i\Delta E_A+\sum_{i=1}^{k}[P_{k,i}s_i]''\frac{\Delta E_A^3}{24}; \quad k=1, 2, \ldots, p. \quad (10)$$

Here

$$[P_{k,i}s_i]''=\left\{\frac{\partial^2P(E,E_{0k})}{\partial^2E}s(E)+\frac{\partial P(E,E_{0k})}{\partial E}\frac{\partial s(E)}{\partial E}+P(E,E_{0k})\frac{\partial^2s(E)}{\partial E^2}\right\}_{E=E_i}.$$

Writing

$$\left.\frac{\partial P(E,E_{0k})}{\partial E}\right|_{E=E_i}=P'_{k,i}; \quad \left.\frac{\partial s(E)}{\partial E}\right|_{E=E_i}=s'_i,$$

and defining the matrices

$$\mathbf{P}'=\begin{vmatrix} P'_{1,1} & 0 & 0 & \cdot & 0 & 0 \\ P'_{2,1} & P'_{2,2} & 0 & \cdot & 0 & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 0 & 0 \\ P'_{p-1,1} & P'_{p-1,2} & \cdot & \cdot & P'_{p-1,p-1} & 0 \\ P'_{p,1} & P'_{p,2} & \cdot & \cdot & P'_{p,p-1} & P'_{p,p} \end{vmatrix}; \quad \mathbf{s}'=\begin{vmatrix} s'_1 \\ s'_2 \\ \cdot \\ \cdot \\ s'_{p-1} \\ s'_p \end{vmatrix},$$

and analogously for higher derivatives, and derivative matrices, the p equations (10) may be written as one matrix equation

$$\mathbf{y}_0 \simeq \Delta E_A \mathbf{P}.\mathbf{s}+(\Delta E_A^3/24)\{\mathbf{P}''.\mathbf{s}+2\mathbf{P}'.\mathbf{s}'+\mathbf{P}.\mathbf{s}''\}. \tag{11}$$

Premultiplying each side of (11) by $(1/\Delta E_A)\mathbf{C}$, one obtains with (4) and (5)

$$\mathbf{s}-\bar{\mathbf{s}}=-(\Delta E_A^2/24)\{\mathbf{C}.\mathbf{P}''.\mathbf{s}+2\mathbf{C}.\mathbf{P}'.\mathbf{s}'+\mathbf{s}''\}.$$

Numerical coefficients of the matrices $\mathbf{C}.\mathbf{P}''$ and $2\mathbf{C}.\mathbf{P}'$ were computed using the spectral distribution function of Penfold and Leiss (1958). It was found that in practical cases an error smaller than 20% in the values of elements of $\mathbf{s}-\bar{\mathbf{s}}$ is introduced if the further approximation

$$\mathbf{s}-\bar{\mathbf{s}} \simeq -(\Delta E_A^2/24)\mathbf{s}'' \tag{12}$$

is used. Equation (12) defines p ordinates $s(E_i)-\bar{s}(E_i)$; $i=1, 2, \ldots, p$, but as the summation (9) may be started at any energy E_{00} between 0 and ΔE_A, all the sets $s(E_i)-\bar{s}(E_i)$, corresponding to all the values E_{00} define a continuous function $s(E)-\bar{s}(E)$, where

$$s(E)-\bar{s}(E)=-\frac{\Delta E_A^2}{24}\frac{\partial^2 s(E)}{\partial E^2}. \tag{13}$$

Assume, for example, that $s(E)$ is a resonance of height S and half-width Γ, and has a Gaussian shape symmetric about E_M, i.e.

$$s(E)=S\exp\left[-4(\ln 2)\frac{(E-E_M)^2}{\Gamma^2}\right],$$

and then with (13)

$$\bar{s}(E)=s(E)+\frac{\Delta E_A^2}{24}\frac{\mathrm{d}^2 s(E)}{\mathrm{d}E^2}$$

$$=s(E)\left\{1-0\cdot230\frac{\Delta E_A^2}{\Gamma^2}+1\cdot281\frac{\Delta E_A^2}{\Gamma^2}\left(\frac{E-E_M}{\Gamma}\right)^2\right\}.$$

$\bar{s}(E)$ has very nearly Gaussian shape, with height $\bar{S}$ and half-width $\bar{\Gamma}$, where

$$\bar{S}=S(1-0\cdot230\Delta E_A^2/\Gamma^2), \tag{14}$$

$$\bar{\Gamma}=\frac{\Gamma}{(1-0\cdot230\Delta E_A^2/\Gamma^2-0\cdot043\Delta E_A^4/\Gamma^4+\ldots)}. \tag{15}$$

Thus, if $\Gamma>\Delta E_A$, it is a very good approximation to write

$$S\Gamma=\bar{S}\bar{\Gamma}.$$

Equations (14) and (15) may be used to estimate the error in $\bar{s}(E)$ for the case of a non-symmetric resonance. If $\Gamma \sim \frac{1}{2}\Delta E_A$, the resonance is " smoothed out " in $\bar{s}(E)$. The " smoothing " effect due to the use of finite differences (with intervals ΔE_A) is demonstrated by an example in Figure 1.

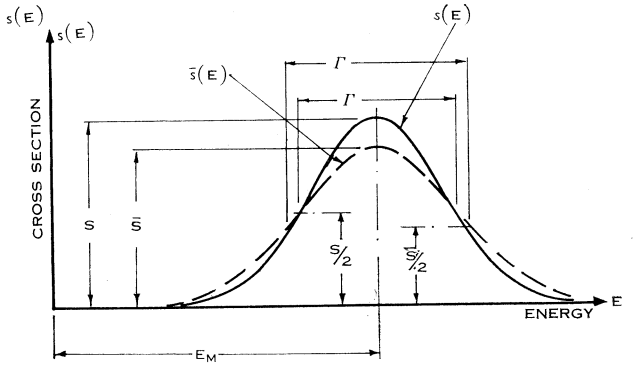

Fig. 1.—Smoothing effect due to the use of finite differences in the yield analysis of a Gaussian resonance. ($\Delta E_A = 0{\cdot}83\Gamma$). $s(E) = S\exp[-4(\ln 2)(E-E_M)^2/\Gamma^2]$, $\bar{s}(E) = s(E) + (\Delta E_A^2/24)\{d^2s(E)/dE^2\}$.

It has been suggested (Cook 1957) that integrated cross sections be computed directly, and that cross sections be found by differentiation. If $\bar{I}_{0k}$ is the directly computed integrated cross section ordinate, corresponding to the exact ordinate $I(E_{0k})$, it is

$$\bar{\mathbf{I}}_0 = \begin{bmatrix} \bar{I}_{01} \\ \bar{I}_{02} \\ \cdot \\ \cdot \\ \bar{I}_{0,p-1} \\ \bar{I}_{0p} \end{bmatrix} = \Delta E_A \begin{bmatrix} 1 & 0 & 0 & \cdot & 0 & 0 \\ 1 & 1 & 0 & \cdot & 0 & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 0 & \cdot \\ 1 & 1 & \cdot & \cdot & 1 & 0 \\ 1 & 1 & \cdot & \cdot & 1 & 1 \end{bmatrix} \cdot \begin{bmatrix} \bar{s}_1 \\ \bar{s}_2 \\ \cdot \\ \cdot \\ \bar{s}_{p-1} \\ \bar{s}_p \end{bmatrix} = \Delta E_A \mathbf{D}.\bar{\mathbf{s}}$$

and with (5)

$$\bar{\mathbf{I}}_0 = \mathbf{D}.\mathbf{C}.\mathbf{y}_0 = \mathbf{F}.\mathbf{y}_0.$$

It is easily verified that, as long as (13) is valid, $\bar{I}_{0k} = I_{0k}$. However, as long as no *a priori* assumption is made about the smoothness of the exact continuous integrated cross section $I(E)$, the cross section derived from the discrete set of ordinates I_{0k} will be in error again by an amount as given by (13). Unless one is particularly interested in the integrated cross section itself, its computation is thus only an unnecessary complication in cross-section computations.

II. Statistical Errors

In general the discrete set of exact yield ordinates $y(E_{0k})$, $k=1, 2, \ldots, p$ is not known. The experiment rather supplies a discrete set of yield ordinates

$$\mathfrak{y}(E_{0k}) \pm \mathrm{st}\,[\mathfrak{y}(E_{0k})]\,; \quad k=1, 2, \ldots p,$$

where st $[\mathfrak{y}(E_{0k})]$ denotes the standard error in $\mathfrak{y}(E_{0k})$. If the set of cross-section ordinates

$$\bar{\mathfrak{s}}(E_k) = \bar{\mathfrak{s}}_k\,; \quad k=1, 2, \ldots, p,$$

is computed from (6), by using in place of ordinates y_{0k} the ordinates $\mathfrak{y}(E_{0k})=\mathfrak{y}_{0k}$, the standard error $\mathrm{st}[\bar{\mathfrak{x}}_k]$ can be computed from (6) by the law of propagation of errors, namely,

$$\mathrm{st}[\bar{\mathfrak{x}}_k]=\frac{1}{\Delta E_A}\left(\sum_{i=1}^{k} C_{k,i}^2\,\mathrm{st}[\mathfrak{y}_{0i}]^2\right)^{\frac{1}{2}}.$$

The coefficients $C_{k,i}$ decrease rapidly with decreasing i. Then if $\mathrm{st}[\mathfrak{y}_{0i}]$ does not vary much for neighbouring values of E_{0k}, a good approximation is

$$\mathrm{st}[\bar{\mathfrak{x}}_k]\simeq\frac{1}{\Delta E_A}\mathrm{st}[\mathfrak{y}_{0k}]\left(\sum_{i=1}^{k} C_{k,i}^2\right)^{\frac{1}{2}}. \tag{16}$$

The square root in (16) was computed for the energy interval

$$5\ \mathrm{MeV}<E_{0p}<25\ \mathrm{MeV}$$

for several values of ΔE_A. It was found that (16) may be approximated for this energy interval by

$$\mathrm{st}[\bar{\mathfrak{x}}_k]\simeq\Delta E_A^{-3/2}E_{0k}\,\mathrm{st}[\mathfrak{y}_{0k}]\cdot\mathrm{const.} \tag{17}$$

The error in $\mathrm{st}[\bar{\mathfrak{x}}_k]$ due to this approximation is smaller than 20%, even in extreme cases.

III. Experimental Resolution

Suppose a cross section $s(E)$ contains several maxima. If $s(E)$ were known, it would be possible in principle to calculate the probability that two particular maxima of $s(E)$ are resolved with statistical significance through a discrete set of experimental cross-section ordinates

$$\bar{\mathfrak{x}}_k\pm\mathrm{st}[\bar{\mathfrak{x}}_k]\ ;\quad k=1,\ 2,\ .\ .\ .,\ p.$$

As $s(E)$ is unknown in practice, it is convenient to use a hypothetical function ${}_Rs(E)$ as a standard analytical function, which contains two maxima, and to investigate under which conditions for p, $\mathrm{st}[{}_R\mathfrak{y}_{0k}]$, and ΔE_A these maxima would be resolved through the corresponding discrete set of computed cross-section ordinates ${}_R\bar{\mathfrak{x}}_k\pm\mathrm{st}[{}_R\bar{\mathfrak{x}}_k]$. Then a quantitative criterion is obtained which indicates the minimum distance between two maxima in a standard function ${}_Rs(E)$, for which the information contained in the corresponding set ${}_R\bar{\mathfrak{x}}_k\pm\mathrm{st}[{}_R\bar{\mathfrak{x}}_k]$ is sufficient to resolve these maxima with statistical significance. This criterion will enable one to decide, at least with reasonable assurance, whether two maxima apparent from some set of experimental ordinates $\bar{\mathfrak{x}}_k\pm\mathrm{st}[\bar{\mathfrak{x}}_k]$ are real, or are only apparent owing to statistical fluctuations. The procedure is analogous to the definition of resolution in the optical case. Here one examines a standard image interference pattern as seen by the imperfect optical system with its finite resolution, and which corresponds to two image points of a perfect optical system, having infinite resolving power.

A function which is the superposition of two symmetric Gaussian resonances, each with height S and half-width Γ is chosen for the standard function ${}_Rs(E)$, that is,

$${}_Rs(E)=S\left\{\exp\left[-4(\ln 2)\left(\frac{E-E_{M1}}{\Gamma}\right)^2\right]+\exp\left[-4(\ln 2)\left(\frac{E-E_{M2}}{\Gamma}\right)^2\right]\right\}. \tag{18}$$

The two maxima at E_{M1} and E_{M2} shall be separated by (see Fig. 2)

$$d=E_{M2}-E_{M1}=1\cdot41165\Gamma\simeq\sqrt{2}.\Gamma.$$

The dip at $E=\frac{1}{2}(E_{M1}+E_{M2})$ is exactly $\frac{1}{2}S$. The corresponding function ${}_R s(E)$ is computed, by making use of equation (13). For the interval

$$E_{M1}<E<E_{M2}, \tag{19}$$

equation (18) may be approximated by

$${}_R s(E)\simeq\tfrac{3}{4}S+\tfrac{1}{4}S\cos[(2\pi/d)(E-E_{M1})],$$

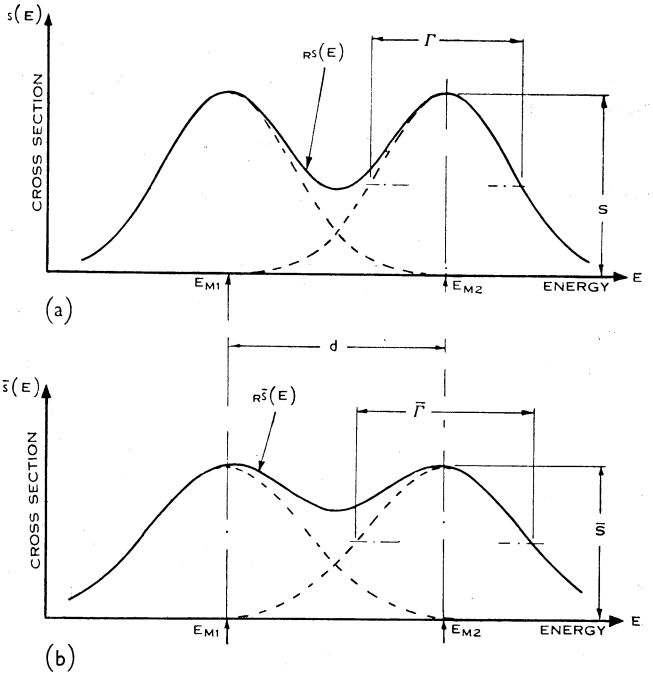

Fig. 2 (*a*).—Standard cross-section ${}_R s(E)$. (Superposition of two Gaussian resonances.)

${}_R s(E)=S\{\exp[-4(\ln 2)(E-E_{M1})^2/\Gamma^2]+\exp[-4(\ln 2)(E-E_{M2})^2/\Gamma^2]\}$.

Fig. 2 (*b*).—Smoothing effect due to the use of finite differences in the yield analysis on ${}_R s(E)$ of Figure 2 (*a*). ($\Delta E_A=0\cdot83\Gamma$).

${}_R\bar{s}(E)={}_R s(E)+(\Delta E_A^2/24)\{d^2{}_R s(E)/dE^2\}$.

and with (13) the corresponding approximation for ${}_R\bar{s}(E)$ becomes

$${}_R\bar{s}(E)=\tfrac{3}{4}S+\tfrac{1}{4}S\left[1-\frac{\Delta E_A^2}{24}\,\frac{4\pi^2}{d^2}\right]\cos\left[\frac{2\pi}{d}(E-E_{M1})\right]. \tag{20}$$

In interval (19) the error due to this approximation is smaller than $0\cdot4\,\%$ for ${}_R s(E)$ and smaller than $1\cdot5\,\%$ for ${}_R\bar{s}(E)$ for $\Delta E_A<\Gamma$. ${}_R s(E)$ and ${}_R\bar{s}(E)$ for $\Gamma=1\cdot2\Delta E_A$ are shown on Figure 2. The dip in ${}_R\bar{s}(E)$ will disappear for $\Delta E_A>1\cdot1\Gamma$.

Suppose now from yield ordinates of a hypothetical experiment cross-section ordinates with standard errors

$$ {}_R\bar{\bar{s}}_k \pm \mathrm{st}[{}_R\bar{\bar{s}}_k]\,; \quad k=1,\ 2,\ .\ .\ .,\ p, $$

were computed, and that of the p ordinates, g ordinates

$$ {}_R\bar{\bar{s}}_f \pm \mathrm{st}[{}_R\bar{\bar{s}}_f]\,; \quad f=1,\ 2,\ .\ .\ .,\ g, $$

lie in the interval defined by (19). If $\Delta E_e = E_{f+1} - E_f$,

$$ g \cdot \Delta E_e \simeq E_{M2} - E_{M1} = d. \tag{21} $$

ΔE_e need not be equal to ΔE_A, but ΔE_A has to be an integral multiple of ΔE_e. For example, E_{0k} may have values 8·00, 8·25, 8·50, 8·75, . . ., 18·00 MeV. Then one may split the corresponding yield ordinates into two groups, one at energies 8·00, 8·50, 9·00, . . ., 18·00 MeV (group I) and the second one at energies 8·25, 8·75, 9·25, . . ., 17·75 MeV (group II), and analyse group I and group II independently with $\Delta E_A = 0{\cdot}5$ MeV. (Here then $\Delta E_e = 0{\cdot}25$ MeV and $\Delta E_A = 2\Delta E_e$.)

It follows from (20) that ${}_R\bar{s}(E)$ has to be of the form

$$ {}_R\bar{s}(E) = A_1 + A_2 \cos\left[(2\pi/d)(E - E_{M1})\right], \tag{22} $$

where A_1 and A_2 are constants. To reconstruct ${}_R\bar{s}(E)$ for the interval (19) from the set of ordinates ${}_R\bar{\bar{s}}_f \pm \mathrm{st}[{}_R\bar{\bar{s}}_f]$; $f=1,\ 2,\ .\ .\ .,\ g$, one has to fit by a Gaussian least square fit to ${}_R\bar{\bar{s}}_f$; $f=1,\ 2,\ .\ .\ .,\ g$, a function

$$ {}_R\hat{\bar{s}}(E) = \hat{A}_1 + \hat{A}_2 \cos\left[(2\pi/d)(E - E_{M1})\right]. \tag{23} $$

The fitting of a curve here is unambiguous, as the analytical form of ${}_R\bar{s}(E)$ is known. Then

$$ \hat{A}_2 = \frac{2}{g} \sum_{f=1}^{g} {}_R\bar{\bar{s}}_f \cos\left[\frac{2\pi}{d}(E_f - E_{M1})\right], $$

and by the law of propagation of errors, the standard error $\mathrm{st}[\hat{A}_2]$ in $\hat{A}_2$ becomes

$$ \mathrm{st}[\hat{A}_2] = (2/g)^{\frac{1}{2}} \mathrm{st}[{}_R\bar{\bar{s}}]. \tag{24} $$

In equation (24) it is assumed, for the sake of simplicity, that standard errors $\mathrm{st}[{}_R\bar{\bar{s}}_f]$ are approximately equal to $\mathrm{st}[{}_R\bar{\bar{s}}]$.

Only if $\hat{A}_2$ is positive will the dip be apparent from (23).

If

$$ \gamma\, \mathrm{st}[\hat{A}_2] = A_2, \tag{25} $$

the chance that the dip is apparent from (23) is approximately 62% for $\gamma=1$, 86% for $\gamma=1{\cdot}5$, etc. With (20) and (22)

$$ A_2 = \tfrac{1}{4} S \left[1 - \frac{\Delta E_A^2}{24} \frac{4\pi^2}{d^2}\right]. \tag{26} $$

Thus the condition that the dip is seen with a chance corresponding to γ is, with (24), (25), and (26),

$$ \gamma \left(\frac{2}{g}\right)^{\frac{1}{2}} \mathrm{st}[{}_R\bar{\bar{s}}] = \tfrac{1}{4} S \left[1 - \frac{\Delta E_A^2}{24} \frac{4\pi^2}{d^2}\right]. \tag{27} $$

Reversing the argument, if $\mathrm{st}[{}_R\bar{\mathfrak{s}}]$, S, and ΔE_A are given, d of (27) is then the minimum separation of two maxima in a cross section of form (18) for which the dip is apparent with statistical significance form $\bar{\mathfrak{s}}_k \pm \mathrm{st}[\bar{\mathfrak{s}}_k]$; $k=1, 2, \ldots, p$. The resolution $r(\gamma, \Delta E_A)$ is then defined by

$$r(\gamma, \Delta E_A)=1/d. \tag{28}$$

Through (27), d and $r(\gamma, \Delta E_A)$ are given as function of γ, g, $\mathrm{st}[{}_R\bar{\mathfrak{s}}]$, and ΔE_A. From experimental data $\mathrm{st}[\bar{\mathfrak{s}}_k]=\mathrm{st}[\bar{\mathfrak{s}}]$ may be computed from (17), but is still a function of ΔE_A. It is convenient to express $\mathrm{st}[\bar{\mathfrak{s}}]$ in terms of a fixed reference value $\Delta E_{A,1}$ (e.g. $\Delta E_{A,1}=1$ MeV). Then with (17)

$$\mathrm{st}[\bar{\mathfrak{s}}]\Delta E_A^{3/2}=\mathrm{st}[\bar{\mathfrak{s}}]_1\Delta E_{A,1}^{3/2}, \tag{29}$$

where $\mathrm{st}[\bar{\mathfrak{s}}]_1$ is the standard error computed from experimental data with $\Delta E_{A,1}$. A parameter which is characteristic of the amount of information contained in a discrete set of experimental yield ordinates $\mathfrak{y}_{0k} \pm \mathrm{st}[\mathfrak{y}_{0k}]$ is then given by

$$\varepsilon_1=\gamma S^{-1}\,\mathrm{st}[\bar{\mathfrak{s}}]_1\Delta E_{A,1}^{3/2}(2\Delta E_e)^{\frac{1}{2}}. \tag{30}$$

Using (27) with (21), (28), (29), and (30) as an equation for $r(\gamma, \Delta E_A)$ in terms of ΔE_A, one obtains

$$r^2(\gamma, \Delta E_A)+\frac{24\varepsilon_1}{\pi^2\Delta E_A^{7/2}}\{r(\gamma, \Delta E_A)\}^{\frac{1}{2}}=\frac{24}{4\pi^2\Delta E_A^2}. \tag{31}$$

Equation (31) is a quartic equation in $\{r(\gamma, \Delta E_A)\}^{\frac{1}{2}}$, in which the parameter ε_1 is independent of ΔE_A. Solutions of d and $r(\gamma, \Delta E_A)$ as function of ΔE_A and ε_1 may be interpolated from Figure 3.

The resolution $r(\gamma, \Delta E_A)$ depends on the choice of ΔE_A in the following way. If ΔE_A is chosen large, the smoothing effect due to the replacement of integration by summation of finite differences (equation (2) replaces (1)) becomes large, and apparent statistical errors (equation (29)) are small. If ΔE_A is chosen small the smoothing effect becomes negligible, but apparent statistical errors become excessively large.

The condition that the resolution $r(\gamma, \Delta E_A)$ has a maximum ($r_{\max.}$), and d has a minimum ($d_{\min.}$) is

$$\frac{\partial r(\gamma, \Delta E_A)}{\partial(\Delta E_A)}=0\,; \quad \frac{\partial^2 r(\gamma, \Delta E_A)}{\partial(\Delta E_A)^2}<0.$$

From equation (31), the value $\Delta E_A=\Delta E_{\mathrm{opt.}}$, corresponding to $r_{\max.}$ and $d_{\min.}$, is given by

$$\left.\begin{aligned} \Delta E_{\mathrm{opt.}}&=2\cdot 236\varepsilon_1^{1/2},\\ r_{\max.}&=0\cdot 2282\varepsilon_1^{-1/2}=0\cdot 5104\Delta E_{\mathrm{opt.}}^{-1},\\ d_{\min.}&=1\cdot 959\Delta E_{\mathrm{opt.}}=4\cdot 472\varepsilon_1^{1/2}. \end{aligned}\right\} \tag{32}$$

If a cross section has exactly the shape of ${}_Rs(E)$ (Fig. 2), the choice of $\Delta E_A=\Delta E_{\mathrm{opt.}}$ would give maximum resolution, but, as in practice $s(E)$ may have a shape quite different from ${}_Rs(E)$, the use of $\Delta E_{\mathrm{opt.}}$ for the cross-section computation need not necessarily ascertain that the maximum amount of information contained in the set $\mathfrak{y}_{0k} \pm \mathrm{st}[\mathfrak{y}_{0k}]$ is expressed in the corresponding set $\bar{\mathfrak{s}}_k \pm \mathrm{st}[\bar{\mathfrak{s}}_k]$.

The choice of ΔE_A is limited to two or three values in any case if the tabulated values $B_{i,n}$ of Penfold and Leiss (1958) (equations (6) and (7)) are used for the yield analysis. It is recommended that cross sections be computed twice independently with the two available values ΔE_A nearest to $\Delta E_{\text{opt.}}$.

ΔE_e is inversely proportional to p, the number of yield ordinates $\mathfrak{y}_{0k}$. $\text{st}[\bar{\mathfrak{s}}_k]$ is inversely proportional to the square root of the number of counts (events) taken, to measure one ordinate $\mathfrak{y}_{0k}$. Then with (30), ε_1 is inversely proportional to the total number of counts taken, to measure all ordinates $\mathfrak{y}_{0k}$, and hence with (32)

$$r_{\text{max.}}=1/d_{\text{min.}} \propto (\text{total number of counts})^{\frac{1}{2}}. \qquad (32a)$$

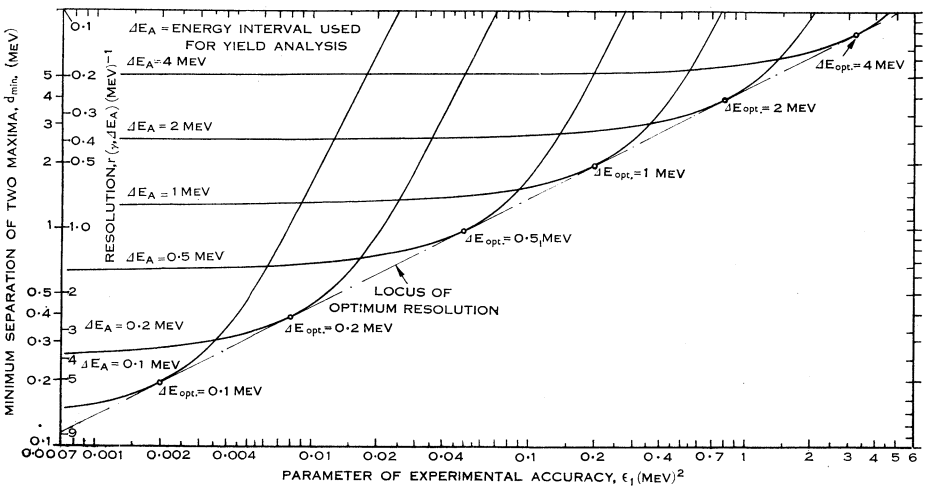

Fig. 3.—Experimental resolution of bremsstrahlung experiments $r(\gamma, \Delta E_A)$, equation (28), as function of experimental accuracy (parameter ε_1, equation (30)).

$$\varepsilon_1=\gamma\ \text{st}[\bar{\mathfrak{s}}]_1 \Delta E_{A,1}^{3/2}(2\Delta E_e)^{\frac{1}{2}}/S \quad (\text{MeV})^2.$$

Suppose, for example, in a bremsstrahlung experiment yield ordinates were measured at 0·25 MeV intervals ($\Delta E_e=0{\cdot}25$ MeV), and with $\Delta E_A=\Delta E_{\text{opt.}}=1$ MeV for the yield analysis the cross section showed evidence for two resonances, 2 MeV apart. If the experimental resolution here was $[2\ \text{MeV}]^{-1}$, ($d=2$ MeV), one would have reasonable assurance that the two observed resonances are real and not due to statistical fluctuations. If in an improved experiment one wants to make certain that the resonances are real one may endeavour to double the experimental resolution. According to (32a), here the total number of counts of the improved experiment has to be 16 times that of the initial experiment. This may be achieved by again measuring yield ordinates at 0·25 MeV intervals, but increasing the number of counts taken to measure individual yield ordinates by a factor of 16. An equivalent alternative would be to measure yield ordinates at for example 0·1 MeV intervals ($\Delta E_e=0{\cdot}1$ MeV) and increase the number of counts of individual yield ordinates by a factor of 6·4. According to (30) and (32) the optimum value of ΔE_A to be chosen for the yield analysis would be the same in either case (here $\Delta E_A=\Delta E_{\text{opt.}}=0{\cdot}5$ MeV).

IV. Smoothing and Curve-fitting

When a physical interpretation is to be given to a discrete set of ordinates with their errors, one will fit subjectively a smooth curve to the set of ordinates. As a matter of fact this process may often consist merely in picturing where the smooth curve would lie without actually drawing the curve. This subjective type of interpolation is not unambiguous if proportional errors are large and the ordinates are spaced widely. The following simple procedure is then often employed. One draws " by eye " a smooth curve with minimum curvature such that the smooth curve cuts only approximately two-thirds of the error bars. This method " smooths out " statistical fluctuations, but may also smooth out a certain amount of information contained in the experimental data.

In the analysis of experimental data, " smoothing by eye " may be applied to yield ordinates, yield first-difference ordinates, integrated cross-section ordinates, or cross-section ordinates. Whichever method is used, finally a continuous " smooth " cross section $\hat{\bar{\mathfrak{s}}}(E)$ is obtained, but the statistical uncertainty in $\hat{\bar{\mathfrak{s}}}(E)$ is only known vaguely (and for this reason is usually not stated in the literature).

The fitting of a " smooth " continuous function may be done analytically, by making a Gaussian least square fit of a set of known functions to the discrete set of ordinates. The statistical uncertainty in the resulting continuous function can be computed in this case.

Suppose, for example, that a set of functions is to be fitted analytically to a discrete set of cross-section ordinates $\bar{\mathfrak{s}}_k \pm \mathrm{st}[\bar{\mathfrak{s}}_k]$; $k=1, 2, \ldots, p$. For the sake of simplicity it will be assumed that all standard errors are equal,* and that ${}^rf(E)$; $r=1, 2, \ldots$, the set of functions to be fitted, is orthonormal in the energy interval

$$E_1 - \tfrac{1}{2}\Delta E_e < E < E_p + \tfrac{1}{2}\Delta E_e, \tag{33}$$

that is,

$$\sum_{k=1}^{p} {}^rf(E_k)\,{}^sf(E_k)\Delta E_e = \delta_{rs} \begin{cases} =1, & r=s \\ =0, & r\neq s \end{cases} \text{(orthonormality condition)} \tag{34}$$

$$\sum_{r=1}^{p} {}^rf(E_j)\,{}^rf(E_k)\Delta E_e = \delta_{jk} \begin{cases} =1, & j=k \\ =0, & j\neq k \end{cases} \text{(closure property)} \tag{35}$$

If the first q functions ${}^rf(E)$ are fitted by a Gaussian least square fit to the p ordinates $\bar{\mathfrak{s}}_k$,

$${}^q\hat{\bar{\mathfrak{s}}}(E) = \sum_{r=1}^{q} {}^r\hat{a}\,{}^rf(E). \tag{36}$$

The constants ${}^r\hat{a}$, which are the same for all values q due to (34), are then found from

$${}^r\hat{a} = \sum_{k=1}^{p} \bar{\mathfrak{s}}_k\,{}^rf(E_k)\Delta E_e, \tag{37}$$

* If $\mathrm{st}[\bar{\mathfrak{s}}_k]$ varies smoothly (or approximately smoothly) with E_k, the case may be reduced to the above one, by forming the function

$$\bar{\mathfrak{z}}_k \pm \mathrm{st}[\bar{\mathfrak{z}}_k] = \bar{\mathfrak{s}}_k/\mathrm{st}[\bar{\mathfrak{s}}_k] \pm \mathrm{st}[\bar{\mathfrak{s}}_k]/\mathrm{st}[\bar{\mathfrak{s}}_k] ;$$

$k=1, 2, \ldots, p$, and treating $\bar{\mathfrak{z}}_k$ as above.

and by the law of propagation of errors, the standard error $\mathrm{st}[{}^{r}\hat{a}]$ in ${}^{r}\hat{a}$ becomes, with (34) and (37),

$$\mathrm{st}[{}^{r}\hat{a}] = \mathrm{st}[\bar{\bar{s}}](\Delta E_e)^{\frac{1}{2}}, \tag{38}$$

and, with (35), (36), and (38), the standard error $\mathrm{st}[{}^{q}\hat{\bar{s}}]$ in each of the p ordinates ${}^{q}\hat{\bar{s}}(E_k) = {}^{q}\hat{\bar{s}}_k$ becomes

$$\mathrm{st}[{}^{q}\hat{\bar{s}}] = \mathrm{st}[\bar{\bar{s}}](q/p)^{\frac{1}{2}}.$$

Then if $q=p$, the function ${}^{q}\hat{\bar{s}}(E) = {}^{p}\hat{\bar{s}}(E)$ will pass exactly through ordinates $\bar{\bar{s}}_k$ and standard errors $\mathrm{st}[{}^{p}\hat{\bar{s}}]$ are identical with $\mathrm{st}[\bar{\bar{s}}]$, the experimental standard errors. If $q<p$, ${}^{q}\hat{\bar{s}}(E)$ is "smoother" than ${}^{p}\hat{\bar{s}}(E)$, i.e. it contains less detail, but the standard errors in the p ordinates ${}^{q}\hat{\bar{s}}_k$ are smaller by a factor of $(q/p)^{\frac{1}{2}}$ than the original standard error $\mathrm{st}[\bar{\bar{s}}]$. In the extreme case $q=1$, ${}^{1}\hat{\bar{s}}(E)$ is just a straight line parallel to the E-axis, at average cross-section height, with $\mathrm{st}[{}^{1}\hat{\bar{s}}] = p^{-\frac{1}{2}}\,\mathrm{st}[\bar{\bar{s}}]$.

One requires the highest value of q for which the fitted continuous curve ${}^{q}\hat{\bar{s}}(E)$ does not show yet apparent detail which is due to statistical fluctuations, and not originally contained in $s(E)$. This value of q may be found rigorously by applying chi-square tests to sets of ${}^{q}\hat{\bar{s}}_k$, $\mathrm{st}[{}^{q}\hat{\bar{s}}_k]$, and $\bar{\bar{s}}_k$ for successive values of q. An adequate criterion is to ascertain that for none of the coefficients ${}^{r}\hat{a}$ used, $\mathrm{st}[{}^{r}\hat{a}] \geqslant {}^{r}\hat{a}$. A curve ${}^{q}\hat{\bar{s}}(E)$ fitted analytically with the highest permissible q value ideally will extract the maximum amount of information contained in the original data, and will in general show more genuine detail than a curve fitted "by eye with minimum curvature". However, analytical curve fitting may not be used unless the permissible number of curves is sufficiently large (say greater than five), and it is ascertained that boundary conditions at the limits of interval (33) do not introduce systematic distortions. ${}^{q}\hat{\bar{s}}(E)$ does not approximate $\bar{s}(E)$ but rather a function ${}^{q}\hat{\bar{s}}(E)$, which would be obtained by fitting q functions to the "exact" ordinates $\bar{s}_k$; $k=1, 2, \ldots, p$. For $q<p$ the function ${}^{q}\hat{\bar{s}}(E)$ will be smoother again, in general, than $\bar{s}(E)$. This smoothing effect is very similar to the smoothing introduced by using a large ΔE_A in the yield analysis (there $s(E) \to \bar{s}(E)$, see Fig. 2).

To indicate the statistical accuracy of a continuous function ${}^{q}\hat{\bar{s}}(E)$, draw the smooth curves ${}^{q}\hat{\bar{s}}(E) + \mathrm{st}[{}^{q}\hat{\bar{s}}]$ and ${}^{q}\hat{\bar{s}}(E) - \mathrm{st}[{}^{q}\hat{\bar{s}}]$. These curves enclose what shall be defined as the "area of statistical variation" of ${}^{q}\hat{\bar{s}}(E)$. The meaning of this area of statistical variation is the following.

Approximately 62% linearly independent points of ${}^{q}\hat{\bar{s}}(E)$ should lie less than $\mathrm{st}[{}^{q}\hat{\bar{s}}]$ above or below ${}^{q}\hat{\bar{s}}(E)$. In the energy interval (33), the number of linearly independent points of ${}^{q}\hat{\bar{s}}(E)$ is q. This may be indicated, e.g. by drawing q error bars with $\mathrm{st}[{}^{q}\hat{\bar{s}}] = \mathrm{st}[\bar{\bar{s}}](q/p)^{\frac{1}{2}}$ equidistant on ${}^{q}\hat{\bar{s}}(E)$. Only such q points can vary independently within statistical limits, and all other points are linearly

dependent. This means effectively that $\hat{\bar{s}}(E)$ has to remain smooth between the q points, and that $\hat{\bar{s}}(E)$ preserves the number of its maxima, minima, and turning points, as the set $\bar{s}_k$; $k=1, 2, \ldots, p$ is varied within statistical limits.

It is of interest to know which value of $(q/p)^{\frac{1}{2}}$ corresponds approximately to the amount of smoothing introduced in " smoothing by eye with minimum curvature ". It was found empirically from examples that this value is of order $\frac{1}{2}$ (see Fig. 4). It appears that the value $(q/p)^{\frac{1}{2}} \sim \frac{1}{2}$ is rather the same, whether

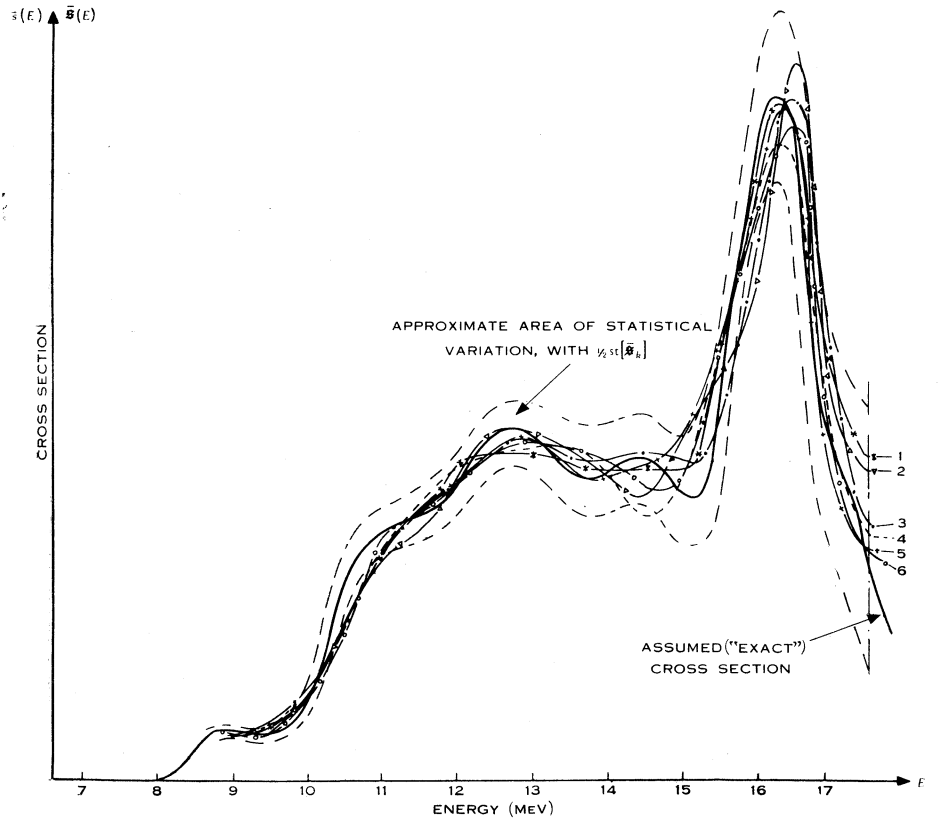

Fig. 4.—Empirical test of " smoothing by eye with minimum curvature " of yield ordinates. Six " experimental " sets of yield ordinates were produced from an assumed (" exact ") set of yield ordinates by a Monte Carlo process. Cross sections 1–6 were obtained by fitting " by eye with minimum curvature " smooth yield curves through the " experimental " yield ordinates and using for the yield analysis the Penfold-Leiss method.

" smoothing by eye with minimum curvature " was applied to yield ordinates or cross-section ordinates, and thus there seems to be no preference for either method. One may obtain an estimate of the statistical accuracy of earlier published cross-section data, if one estimates $\mathrm{st}[\bar{s}_k]$ from standard errors of corresponding yield data, and draws an " approximate area of statistical variation " with $\frac{1}{2}\mathrm{st}[\bar{s}_k]$ above and below the published cross-section curve.

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