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Absorption Spectrometer

by

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The measured response at any absorber \( m \) can be represented by the integral

\[
S_m = \int_0^{E_{\text{max}}} M(m, E) R(E) \sigma(E) dE
\]

where \( R(E) \) is the relative response of the detector at photon energy \( E \), \( \sigma(E) \) is the spectral energy density, and \( M \) is the transmission of the absorber identified by index \( m \) at energy \( E \). It is convenient to simulate the spectrum by a histogram, which allows integration over portions of the spectrum in which the absorption cross section is changing rapidly. Thus it is assumed that the spectral intensity and the detector response are constant over an interval \( E_0 \). If \( R_k \sigma_k \) is taken as the height of the \( k \)-th step of the histogram (uncorrected for detector response), we then have

\[
(S_m) = (M_{mk})(R_k \sigma_k)
\]
when the matrix element $M_{mk}$ is given by

$$M_{mk} = \langle e^{-\mu_m x_m} \rangle$$

$$= \frac{(k + \frac{1}{2})E_0}{(k - \frac{1}{2})E_0}$$

Here $\mu_m$ is the absorption coefficient of material $m$ with thickness $x_m$. As an example, the matrix for $E_0 = 50$ keV and the indicated absorbers, obtained by log-log interpolation from Evans's data, is displayed as Table I.

Direct inversion of the matrix is not a practical procedure because the problem is "badly posed"; the results of direct inversion tend to have unphysical values because the inversion procedure is oversensitive to errors in the data. For this reason inversion has been accomplished in an approximate way by first fitting the response points to a rough polynomial capable of representing the data in broad outline. The function used was

$$R\sigma = N[1 - \varepsilon + a(1 - \varepsilon)^5 + (1 - a)(1 - \varepsilon)^{16}]$$

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<table>
<thead>
<tr>
<th>STEP NO. (m)</th>
<th>MATERIAL</th>
<th>THICKNESS (CM)</th>
<th>ENERGY INCREMENT (k)</th>
<th>CENTER ENERGY (KEV)</th>
<th>50</th>
<th>100</th>
<th>150</th>
<th>200</th>
<th>250</th>
<th>300</th>
<th>350</th>
<th>400</th>
<th>450</th>
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<td>1</td>
<td>Clear</td>
<td>----</td>
<td></td>
<td></td>
<td>1</td>
<td>1</td>
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<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
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<tr>
<td>2</td>
<td>Cu</td>
<td>0.043</td>
<td>0.3515</td>
<td>0.8260</td>
<td>0.9155</td>
<td>0.9410</td>
<td>0.9513</td>
<td>0.9578</td>
<td>0.9617</td>
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<td>0.9667</td>
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<tr>
<td>3</td>
<td>Cu</td>
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<td>0.0363</td>
<td>0.3900</td>
<td>0.6377</td>
<td>0.7327</td>
<td>0.7748</td>
<td>0.8021</td>
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<td>0.8314</td>
<td>0.8410</td>
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<td>0.0642</td>
<td>0.1934</td>
<td>0.3768</td>
<td>0.6114</td>
<td>0.7420</td>
<td>0.8192</td>
<td>0.8635</td>
<td>0.8926</td>
<td>0.9115</td>
<td>0.9252</td>
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<tr>
<td>5</td>
<td>Pb</td>
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<td>0.0075</td>
<td>0.0415</td>
<td>0.1263</td>
<td>0.3441</td>
<td>0.5227</td>
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<tr>
<td>6</td>
<td>Pb</td>
<td>0.152</td>
<td>0.0099</td>
<td>0.0093</td>
<td>0.0390</td>
<td>0.1809</td>
<td>0.3515</td>
<td>0.4950</td>
<td>0.5956</td>
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<td>7</td>
<td>Pb</td>
<td>0.216</td>
<td>0.0001</td>
<td>0.0020</td>
<td>0.0114</td>
<td>0.0902</td>
<td>0.2275</td>
<td>0.3687</td>
<td>0.4791</td>
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<td>8</td>
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<td>0.0004</td>
<td>0.0023</td>
<td>0.0400</td>
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<td>0.0163</td>
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</table>
where $a$ is a shape parameter, $\epsilon$ is the ratio of photon to electron energy, and the normalizing constant $N$ is so chosen that all the $R\sigma$'s at multiples of $E_0$ add up to 1. Obviously many other functions could be chosen to give this first approximation. The high order of the polynomial is intended to allow the function to change rapidly at small $\epsilon$'s.

The first-approximation spectrum arrived at in this or some other way can be refined by a least-squares procedure. The fit-refining process, which if carried far enough will of course lead to the same unphysical and unstable results as does the direct inversion of the absorption matrix, can be stopped at any point where such behavior begins to be seen. On examination of the matrix one can get an idea of the upper limit of any $R\sigma$ which can contribute to the response $S$; for example, if there are no responses beyond $m=7$, say, there can be very little radiation above about 200 keV in energy. In such cases, for which it is known that there is negligible spectral density above a given energy it is obviously to no avail to manipulate any $R\sigma$-values above this energy. This therefore limits the number of adjustable parameters to something below the number of data points and so should lead to a stable solution automatically. In other cases, for which it can be inferred visually from the data that
there is a wider spectrum, one can still get stable approximations either by limiting the number of spectral points manipulated or by stopping the process when convergence is no longer obtained.

To understand the procedure involved, suppose we have a set of trial responses \( \tilde{S}_m \), where we take \( R_k \sigma_k \) to be variable and the other \( R_n \sigma_n, n \neq k \), to be fixed in relative value so that

\[
\tilde{S}_m = M_{mk} R_k \sigma_k + \lambda \sum_{n \neq k} M_{mn} R_n \sigma_m = M_{mk} R_k \sigma_k + \lambda Q_{mk},
\]

\[
\lambda \sum_{n \neq k} \sigma_n + \sigma_k = 1,
\]

the normalization being such that the response through the open section of the filter (top row of the matrix) is unity. Now define

\[
\delta = \sum_m \left( \tilde{S}_m - S_m \right)^2 = \sum_m \left( M_{mk} R_k \sigma_k + \lambda Q_{mk} - S_m \right)^2;
\]

the condition \( \delta \frac{\partial \delta}{\partial (R_k \sigma_k)} = 0 \) then gives

\[
R_k \sigma_k = \left[ \sum M_{mk} \left( M_{mk} - Q_{mk} \right) \right]^{-1} \left[ \sum S_m \left( M_{mk} - Q_{mk} \right) \right] - \lambda \sum_m Q_{mk} \left( M_{mk} - Q_{mk} \right)
\]

\[
\sum_{n \neq k} \sigma_n
\]

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using the value of \( \lambda \) provided by the normalization gives finally

\[
R_k^\sigma_k = \frac{\sum_m S_m \left( \frac{M_{mk} - Q_{mk}}{\sum_{n \neq k} \sigma_n} \right) - \left( \sum_{n \neq k} R_n^\sigma_0 \right)^{-1} \sum_m Q_{mk} \left( \frac{M_{mk} - Q_{mk}}{\sum_{n \neq k} \sigma_n} \right)}{\sum_m M_{mk} \left( \frac{M_{mk} - Q_{mk}}{\sum_{n \neq k} \sigma_n} \right) - \left( \sum_{n \neq k} R_n^\sigma_0 \right)^{-1} \sum_m Q_{mk} \left( \frac{M_{mk} - Q_{mk}}{\sum_{n \neq k} \sigma_n} \right)}
\]

To summarize the procedure: we have an initial approximation \( R_k^\sigma_0, R_{n \neq k}^\sigma_{(n \neq k)_0} \); we then get a better approximation (the best obtainable by varying \( \sigma_k \) only) given by \( R_k^\sigma_k \), \( \lambda R_{n \neq k}^\sigma_{(n \neq k)} \). In evaluating \( Q_{mk} \) we note that

\[
Q_{mk} = \tilde{S}_{m0} - M_{mk} R_k^\sigma_0, \quad \sum_{n \neq k} R_n^\sigma_0 = 1 - R_k^\sigma_0, \quad \lambda = \frac{1 - R_k^\sigma_k}{1 - R_k^\sigma_0},
\]

where the zero subscript denotes an initial value (before variation).
REFERENCES


TABLE I

I. Spectrometer Matrix.