Short Communication

Contributions intended for publication under this heading should be expressly so marked; they should not exceed about 1000 *words; they should be forwarded in the usual way to the appropriate Co-editor; they will be published as speedily as possible.*

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On the calculation of transmission factors.

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The use of three-dimensional parabolic integration is proposed for the calculation of transmission factors. The method does not make use of a grid (isometric or otherwise) to represent the crystal. Typical computing time is 0·1 second per reflexion on a CDC 6600 computer.

The transmission factor A^{-1} is given by

$$A^{-1} = V^{-1} \int \exp\left[-(l_i + l_d)\mu\right] \mathrm{d}V \,, \qquad (1)$$

where V is the irradiated crystal volume, μ is the linear absorption coefficient, and l_i and l_d denote the path lengths of the incident and diffracted beams respectively. Equation (1) may be evaluated numerically (Busing & Levy, 1957; de Graaff, 1973) or analytically (de Meulenaer & Tompa, 1965).

In his review on different methods of correction for absorption Coppens (1970) points out that the analytical approach is to be preferred to Gaussian quadrature for transmissions of less than 75%, if the accuracy required is 1%. Although the Monte Carlo method can be used profitably (Elemans & Verschoor, 1973), Coppens' observations still hold for transmission factors below 40% to be calculated with an accuracy of 1% or better.

A step common to both numerical methods mentioned is the division of the crystal into volume elements. Within each element the path lengths l_i and l_d are considered constant. For heavily absorbing crystals this approximation necessitates the use of very many grid points. Consequently the computing time for the Monte Carlo method is roughly inversely proportional to the square of the transmission factor as well as to the maximum variance allowed in the result.

The method we suggest does not have this built-in defect. A program has been written in Fortran IV using three-dimensional parabolic integration to evaluate (1). The Cartesian system in which the integration is carried out is used to describe the crystal in terms of its boundary planes. A typical calculation for a crystal with ten faces and a transmission varying between 60 and 30% took about 0·1 second per reflexion on a CDC 6600 computer. The accuracy in the calculations was 0·5%. A similar calculation for a crystal with about 10% transmission took 0·35 seconds per reflexion.

The results for Cahen & Ibers's (1972) test crystal are tabulated in Table 1. To calculate this table took about eight seconds. These results clearly show that the program performs reasonably well, even for the excessively large absorption effects considered in Table 1. Furthermore, while for heavily absorbing crystals ($A^{-1} < 15\%$) the analytical method is the more efficient one, the algorithm we propose has none of its inherent sensitivities.

Table 1. *Transmission factors of a test crystal calculated by our program and by Cahen & Ibers* (1972)

Reflexions	x (cm)	μ (cm^{-1})	A^{-1} (program)	A^{-1} (C&I)
$\bar{1}10$	1	0·1	0·936	0·937
		1	0·567	0·568
		10	0·094	0·095
		100	0·0096	0·00995
$\bar{1}10$	0·05	1	0·966	0·967
		10	0·735	0·736
		100	0·180	0·180
		1000	0·0191	0·0198
$1\bar{1}0$	1	0·1	0·935	0·936
		1	0·528	0·528
		10	0·020	0·020
		100	0·0002	0·0002
$1\bar{1}0$	0·05	1	0·966	0·967
		10	0·721	0·722
		100	0·077	0·077
		1000	0·0008	0·0008

The program is available on request in CDC and IBM versions. I am indebted to Mr W. J. Vermin for his helpful suggestions concerning the mathematics of the program. All calculations were done on the CDC 6600 computer of the ECN, Petten.

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