hydrone, both charge-transfer interaction and hydrogen bonding are optimized in the 1:1 structure, so it is not surprising that there is no 2:1 complex in this case.

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Short Communications

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. Publication will be quicker if the contributions are without illustrations.*

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A comparison of analytical and numerical methods for the evaluation of the absorption correction in crystal structure analysis.[*]

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A comparison is made between analytical evaluation of the absorption correction using Howells polyhedra and numerical calculation with the Gaussian method. It is shown that convergence can be reached with the numerical method, provided a sufficiently fine grid is chosen. When absorption is large (*i.e.* > 70–80 %) the analytical method is to be preferred as it produces the required accuracy in a much smaller amount of computer time.

An analytical method of evaluating the absorption correction in crystal structure analysis has been described recently (de Meulenaer & Tompa, 1965). The only completely general method available previously was introduced by Busing & Levy (1957) and is based on a numerical evaluation of $\int \exp(-\mu L)dV$ (see also Coppens, Leiserowitz & Rabinovich, 1965). The accuracy of this method depends evidently on the formula and the number of points used. Busing & Levy claim specifically a precision of 0·2 % for transmissions between 50 and 62 % using Gauss's formula and an $8 \times 8 \times 8$ grid and it is intuitively clear and easy to verify that for a constant grid the accuracy decreases with increasing absorption coefficient μ. Clearly, any desired accuracy can be obtained by using finer grids, but it is the purpose of this note to point out that great care must be taken to verify that the number of points used is sufficient for the desired accuracy, and that the computation effort required may become prohibitive.

We have recomputed, using the analytical method, the transmission for some of the reflexions of a needle-shaped crystal of $YFeO_3$ ($\mu = 878 \cdot 8$ cm^{-1} for Cu $K\alpha$ radiation) investigated recently (Coppens & Eibschütz, 1965) and find values differing from those obtained by the Busing & Levy method using a $12 \times 12 \times 32$ grid. We have, therefore, repeated the computation on a finer grid and have obtained values which converge towards those of the analytical method, as shown in Table 1.

Table 1. *Transmission of some reflexions of a crystal of* $YFeO_3$ (*Coppens & Eibschütz,* 1965) *computed by Gaussian integration on the grids indicated and by the analytical method of de Meulenaer & Tompa* (1965)

hkl	$12 \times 12 \times 32$	$24 \times 24 \times 32$	$32 \times 32 \times 32$	Analytical
025	0·0463	0·0378	0·0387	0·0390
$0\bar{2}5$	0·0463	0·0378	0·0387	0·0390
125	0·0375	0·0335	0·0339	0·0340
$1\bar{2}5$	0·0377	0·0332	0·0337	0·0339
225	0·0613	0·0583		0·0587
$2\bar{2}5$	0·0541	0·0509		0·0514
325	0·0695	0·0681		0·0684

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Table 2. *Transmission of a specified reflexion of a rectangular 'crystal' computed by Gaussian integration on the grids indicated and by the analytical method of de Meulenaer & Tompa* (1965), *for different values of the absorption coefficient μ and with the axes of coordinates parallel to the sides of the rectangle*

	n						
μ	6 × 6	8 × 8	12 × 8	24 × 12	32 × 16	48 × 24	Analytical
1	0·3177	0·3179	0·3176				0·3176
2	0·1564	0·1567	0·1566				0·1566
5	0·0542	0·0547	0·0549				0·0549
10	0·0223	0·0252	0·0254	0·0256			0·0256
20		0·0099	0·0100	0·0123	0·0124		0·0124
50			0·0009	0·0035	0·0046	0·0048	0·0048
100				0·0005	0·0015	0·0023	0·0024

Table 3. *Transmission of a specified reflexion of a rectangular 'crystal' computed by Gaussian integration on the grids indicated and by the analytical method of de Meulenaer & Tompa* (1965), *for different values of the absorption coefficient μ and with the axes of coordinates parallel to the incident and diffracted beams*

	n						
μ	6 × 6	8 × 8	12 × 12	24 × 24	32 × 32	48 × 48	Analytical
1	0·3338	0·3135	0·3159	0·3178	0·3182	0·3176	0·3176
2	0·1659	0·1547	0·1559	0·1569	0·1571	0·1566	0·1566
5	0·0593	0·0546	0·0548	0·0552	0·0552	0·0548	0·0549
10	0·0257	0·0257	0·0258	0·0259	0·0259	0·0255	0·0256
20	0·0067	0·0107	0·0125	0·0125	0·0125	0·0123	0·0124
50		0·0013	0·0038	0·0049	0·0049	0·0048	0·0048
100			0·0007	0·0024	0·0024	0·0024	0·0024

This discrepancy is no doubt due to the fact that the derivative of the integrand is not a continuous function and simple one-dimensional tests confirm the lack of precision of methods of numerical integration in such cases. We have also carried out computations on a two-dimensional model: two Busing–Levy-type programs were written for the IBM 1620 machine to compute absorption corrections for a rectangular 'crystal'; the axes of coordinates for the integration were taken parallel to the sides of the rectangle in the first program and parallel to the incident and diffracted rays in the second. A crystal with edges $a = 2{\cdot}228$, $b = 1{\cdot}114$ was used, the incident ray made an angle of arc tan 0·4 with **b** and the diffracted ray the same angle with **a**; the absorption coefficient μ and the grid of the Gaussian integration formula were varied systematically. Tables 2 and 3 show some results obtained with the two programs together with the analytical values.

For a given number of points the result is seen to depend on the choice of axes, unless convergence has been reached.

Thus, great care must be taken in using Gaussian integration formulae when absorption is large, and though the values converge to the analytical values the convergence is often slow and occasionally rather erratic. Ultimate convergence is, of course, assured by the quadratic integrability of the functions concerned (Lanczos, 1956), but the numerical effort required may be prohibitively costly in terms of computer time. The three-dimensional computation of the values on the 32 × 32 × 32 grid quoted in Table 1 took 12 minutes per reflexion on a CDC 1604 computer, while the analytical evaluation took only about 2 minutes per reflexion on the much slower IBM 1620 computer.

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Lattice dimensions with the Polaroid-Land cassette.

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Lattice constants can be determined routinely to better than 1:1000 from single crystals by use of a precession camera equipped with a Polaroid cassette.

The Polaroid X-R7 Land diffraction cassette has proved capable of providing lattice dimensions not only rapidly, but with an accuracy of better than 1:1000 with normal care.

With no corrections for differences in shrinkage or other distortion, we find the reproducibility of distances measured on a series of precession photographs recorded with the Polaroid cassette is of the order of 1:2000 in a distance of