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*

μ	n: 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*

μ	n: 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 $a=2·228$, $b=1·114$ 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

Table 1. *Reproducibility of lattice constant measurements*

All lattice constant calculations are based on the magnification factor $F\lambda = 42{\cdot}737$ Å.mm, as determined empirically from the $Pb(NO_3)_2$ measurements.

Substance	Film no.		r.m.s. fractional deviation	Maximum fractional deviation	Lattice constants (Å) Measured	Lattice constants (Å) Literature
$Pb(NO_3)_2$	1	*a*	0·00056	0·0007		
	2	*a*	0·00026	0·0009		21 °C
	3	*a*	0·00057	0·0012	(7·8566)	$7{\cdot}8566\begin{pmatrix}+9\\-6\end{pmatrix}$
	4	*a*	0·00067	0·0012		(*International Tables*, 1962)
	5	*a*	0·00046	0·0010		
NaCl	1	*a*	0·00062	0·0013		21 °C
	2	*a*	0·00062	0·0012	5·640	$5{\cdot}6403\begin{pmatrix}+5\\-9\end{pmatrix}$
	3	*a*	0·00067	0·0010		*International Tables*, 1962)
Bent KCl crystal	1	a_1	0·00029	0·0005		
		a_2	0·00019	0·0003	$a_1 = 6{\cdot}292$	21 °C
					$a_2 = 6{\cdot}280$	$a = 6{\cdot}29289(\pm 8)$
	2	a_1	0·00039	0·0006	$a_3 = 6{\cdot}279$	(Hambling, 1953)
		a_3	0·00057	0·0008		
$9Al_2O_3.B_2O_3$	1	*a*	0·00030	0·0004		
		b	0·00025	0·0003		
	2	*a*	0·00058	0·0007		
		c	0·00035	0·0006	$a = 5{\cdot}678$	$a = 5{\cdot}65(\pm 3)$
					$b = 15{\cdot}02$	$b = 14{\cdot}98(\pm 10)$
	3	*a*	0·00022	0·0004	$c = 7{\cdot}697$	$c = 7{\cdot}68(\pm 5)$
		b	0·00031	0·0006		(Scholze, 1956)
	4	*a*	0·00044	0·0008		
		c	0·00020	0·0003		

roughly 5 cm, as shown by the typical data in Table 1. Obviously then, a calibration of the apparatus with a standard substance will lead to lattice constants accurate to 1:1000.

All crystals used in this work were about 0·1 mm in diameter, alignment errors were carefully reduced to less than 5 minutes of arc, and molybdenum radiation was used exclusively. It was necessary to wedge a piece of shim stock in the track of the cassette mounting to correct an undesirably loose fit and the cassette was not removed from the camera between exposures. Ambient temperature was maintained between 19° and 23 °C.

The prints were carefully measured on a standard Supper film measuring device. On each film the distances between parallel rows of reflections were measured and the average was calculated for symmetrically equivalent distances on all films from the same substance. Fractional deviations referred to in Table 1 are deviations of individual measurements from this average.

Presumably the high precision of the measurements is due to the dimensional stability of the image formation process: the thin emulsion of the negative is pressed tightly against the fluorescent screen by an air pillow, and the image transfer to the print is semi-dry. Normal variations of temperature and humidity have a minor effect on the dimensional qualities of the prints. A remeasurement of seven of the prints after a period of three months showed the same reproducibility of distances measured on a series of prints, accompanied by a systematic shrinkage of all prints by approximately 1:1000.

It is apparent that greater accuracy can be obtained by recording a calibration pattern on each print together with the sample pattern and by using an accurate travelling microscope for the measurements.

As an adjunct to structure determination this method could often be used to obtain moderately precise lattice constants from the same crystal used for collecting intensity data (with obvious advantages of consistency). Examples of other uses are illustrated by the data in Table 1 for a bent potassium chloride crystal and $9Al_2O_3 . 2B_2O_3$. The latter was a small needle-like crystal found in a preparation believed to be pure corundum crystals; it was identified as $9Al_2O_3 . 2B_2O_3$ by its lattice constants.

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