Forms	φ	ϱ
110	50° 04′	90° 00′
011	3° 31′	30° 32′
121	32° 17′	54° 03′
$\bar{1}21$	330° 22′	53° 23′
$\bar{1}11$	311° 19′	41° 29′
111	51° 37′	43° 08′
100	90° 00′	90° 00′
$\bar{2}11$	293° 07′	56° 09′
120	31° 08′	90° 00′

Forms in order of development: 110, 011, 121, $\bar{1}21$, $\bar{1}11$, 111, 100, $\bar{2}11$, 120.

$$a:b:c = 0{\cdot}8370:1:0{\cdot}5845\,.$$

$X_0' = 0{\cdot}0367$, $\mu = 2°\ 06'$, $\beta = 92°\ 06'$, $d = 59°\ 31'$, $f = 53°\ 43'$.

The Barker setting coincides with Groth's setting and with the cell derived from röntgenographic data.

Barker angles:

$cr = 34°\ 11'$, $za = 53°\ 43'$, $\underline{am} = 39°\ 56'$, $bq = 59°\ 31'$.

(c) *Papaverine bromhydrate*

Isomorphous with papaverine chlorhydrate.

Forms	φ	ϱ
110	50° 07′	90° 00′
120	31° 01′	90° 00′
100	90° 00′	90° 00′
011	3° 58′	30° 08′
111	51° 52′	43° 08′

Forms in order of development: 110, 120, 100, 011, 111.

$$a:b:c = 0{\cdot}8314:1:0{\cdot}5789$$

$X_0' = 0{\cdot}0405$, $\mu = 2°\ 19'$, $\beta = 92°\ 19'$, $d = 59°\ 56'$, $f = 53°\ 36'$.

Here, too, the Barker setting coincides with Groth's setting and with the röntgenographic cell.

Barker angles:

$cr = 34°\ 05'$, $za = 53°\ 36'$, $\underline{am} = 39°\ 53'$, $bq = 59°\ 56'$.

2. X-ray data

Laue diagrams of all three substances confirmed the symmetry as derived from the goniometric measurements.

The given values of the angle β were calculated from the goniometric measurements and from zero-layer Weissenberg diagrams, taken with the b axis as rotation axis (Cu $K\alpha$ radiation). The dimensions of the unit cell (Table 1) were determined from rotation and Weissenberg photographs about all three axes.

Table 1

	a (Å)	b (Å)	c (Å)	β	V (Å^3)	σ_c	Z
Papaverine	9·50	29·22	6·35	—	1805	1·248	4
Papaverine.HCl	13·10	15·80	9·22	92° 36′	1902	1·312	4
Papaverine.HBr	13·82	15·94	9·28	92° 36′	2042	1·350	4

σ_c = calculated density; Z = number of molecules in cell.

Papaverine gives sytematic extinctions for $h00$ with h odd, $0k0$ with k odd and $00l$ with l odd; therefore the space group is $P2_12_12_1$.

Both other isomorphous derivates give absences for $h0l$ with l odd and $0k0$ with k odd. The space group is therefore $P2_1/c$. Determination of the structure is in progress.

We thank Dr A. Van Ryssen who synthetized the substances examined.

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A nomogram for evaluating the temperature factor.*

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The nomogram evaluates the expression

$$\exp\,[(-2B\sin^2\theta)/\lambda^2] = f_t/f_0\,,$$

where the symbols have the usual significance. It has four scales, A, B, C and D. A and D are logarithmic scales with 1 cycle = 10 in.; they are equidistant from C, which is the logarithmic scale having 2 cycles = 10 in. required for multiplication. Since

$$f_t = f_0 \exp\,[(-2B\sin^2\theta)/\lambda^2]$$
$$= f_0 10^{-\frac{2B}{\log_e 10}\cdot\frac{\sin^2\theta}{\lambda^2}} = f_0 10^{-\frac{B}{1{\cdot}15}\cdot\frac{\sin^2\theta}{\lambda^2}}\,,$$

the D scale has its origin displaced to the left, so that the reference line carrying the origins of the A and C scales cuts the D scale at the value 1·15. Thus, if the value of $(\sin^2\theta)/\lambda^2$ is found on the A scale, and the value of $B = 8\pi^2\bar{u}^2/3$ is found on the D scale, the line joining these points will cut the C scale at the point $(B/1{\cdot}15) \times (\sin^2\theta)/\lambda^2$. The antilogarithm of this value is now required, and the B scale, which is a linear inch scale, performs this operation against the A scale. Note that the values on the B scale increase from right to left,

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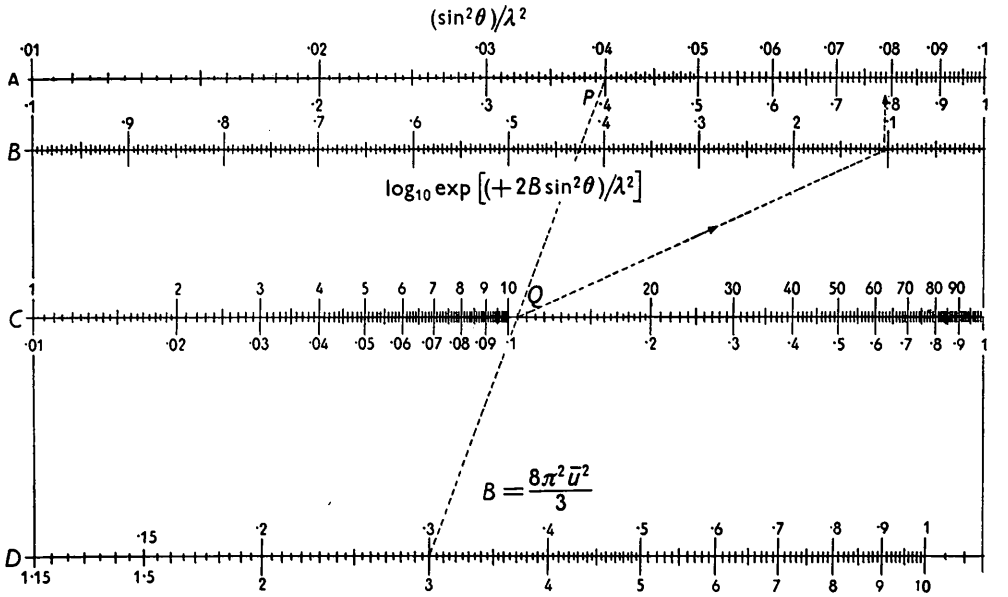

Fig. 1. Nomogram for evaluating $f_t/f_0 = \exp[(-2B\sin^2\theta)/\lambda^2]$. (Reproduced one-half full size.)

because the original equation contains the exponent with a negative sign. An example of the use of the nomogram for evaluating f_t/f_0 for particular values of B and $(\sin^2\theta)/\lambda^2$ has been sketched on the diagram: if $\sin^2\theta/\lambda^2 = 0{\cdot}04$ and $B = 3$, $f_t/f_0 = 0{\cdot}79$, which is the A-scale reading corresponding to the value of Q $(= 0{\cdot}105)$ on the B-scale.

In circumstances in which the temperature factor is assumed to be the same for all the atoms present, the nomogram can be used to evaluate it in the following way. If structure factors, $F_{calc.}$, are calculated using the values of the atomic scattering factors for the atoms at rest, f_0, and a series of values of the ratio $\Sigma|F_{obs.}| \div \Sigma|F_{calc.}|$ is obtained from successive groups of reflections having a mean value of $(\sin^2\theta)/\lambda^2 = M$, then the value of each such ratio, when found on the A scale, determines a point on the B scale and hence a point on the C scale. If the points on the C scale for each value of M are joined to the corresponding values of $(\sin^2\theta)/\lambda^2$ on the A scale, these lines like PQ, when produced, should converge on a particular value of the temperature factor B, which is thereby determined.

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The measurement and correction of intensities from single-crystal X-ray photographs: correction.

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It has been brought to our attention by Mr G. J. Bullen of the Chemistry Department, University College, London, that in our paper (Kaan & Cole, 1949) symbols are used in other than their conventional meanings and that an error occurs in equation (6). These mistakes can be corrected as follows. Throughout the text γ should read Υ and ξ should read ζ. It should be noted that for rotation and oscillation photographs μ is to be replaced by ν, the angle between the diffracted beam and the equatorial layer, as used by Buerger (1942). The definition of Υ given applies strictly to rotation and oscillation photographs only; that for equi-inclination Weissenberg photographs is more general, being the angle between the projections of the direct beam and of the reflected ray on a plane normal to the rotation axis. In both instances Υ is as used by Buerger (1942). The corrected form of equation (6) is

$$\frac{1}{L} = \cos\nu\sin\Upsilon = \sin\Upsilon(1-\zeta^2)^{\frac{1}{2}} = \sin 2\theta\frac{(\sin^2\varrho-\sin^2\theta)^{\frac{1}{2}}}{\cos\theta}.$$

These corrections do not affect the published charts (Figs. 4 and 5) or their use.

Our thanks are due to Mr Bullen for kindly pointing out the above errors.

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