very feeble piezoelectricity but also directly witness the polarity of the phenomenon. The polarity may be deduced by comparing the oscillograms obtained by pressing the crystal first on one side and then on the opposite side. We see, for example, that a phase shift of just 180° takes place in the oscillograms of tourmaline pressed in this way (Fig. 1(*a*), (*b*)). The polarity is further evidenced



Fig. 1. Oscillograms of tourmaline (a) on a face (00.1); (b) on the face opposite to (a); (c) two slips (00.1) superimposed, the same sides of (00.1) being in contact; (d) two slips (00.1)superimposed, the different sides of (00.1) being in contact.

by the test as follows: We cut the specimen into two parts and exert the pressure on them, superimposing them so that first the same and then the different sides come into contact. Whereas with the latter arrangement we obtain an oscillogram (Fig. 1(d)) identical with one of the single slips, with the former we observe that the charge has vanished, the two opposing charges being compensated (Fig. 1(c)). This test is especially useful when the charge developed is very small and we cannot

Acta Cryst. (1953). 6, 664

electricity. We have determined thus that harmotome, $Ba_2Si_{12}Al_4O_{32}$. 12 H₂O, is definitely, though very weakly, piezoelectric.

tell with certainty that it actually arises from piezo-

The method can be used on any tiny crystal fragment to which the pressure head (needle) of the vibrator can be applied. (This may eventually be manipulated under a microscope.) Usually crystal fragments are embedded in resin or other suitable matrix and a slip is made so that two parallel faces are cut or ground from a single fragment.

We have worked also with Cady's and Giebe & Scheibe's 'click' phenomena (Cady, 1922; see also Cady, 1946, p. 231; Giebe & Scheibe, 1925) displayed visually.* The test described above has, however, proved to be much more convenient and satisfactory.

The writer wishes to express his gratitude to Prof. Ito, who has given him guidance and encouragement throughout the present work.

References

BERGMANN, L. (1935). Phys. Z. 36, 31.

- CADY, W. G. (1922). Proc. Inst. Radio. Engrs., N.Y. 10, 83.
- CADY, W. G. (1946). Piezoelectricity. New York: McGraw-Hill.

GIEBE, E. & SCHEIBE, A. (1925). Z. Phys. 33, 760.

* Such a device has been developed at Prof. Hägg's laboratory in Uppsala (private communication from Prof. Ito).

Unit cell and space group of papaverine, papaverine chlorhydrate and papaverine bromhydrate. By A. VAN HULLE, S. AMELINCKX and W. DEKEYSER, Geologisch Instituut, Afdeling Kristalkunde, Rozier 6, Gent, Belgium

(Received 17 April 1953)

1. Goniometric measurements

Papaverine or 6:7-dimethoxy-1-[3':4'-dimethoxy-benzyl] isoquinoline (C₂₀H₂₁O₄N) is an alkaloid of the isoquinoline group (*Beilsteins Handbuch*, 1935). Suitable crystals for examination were obtained by slow evaporation of a solution in alcohol and water.

Some information concerning crystallographic data of the three substances cited above is to be found in Groth (1906–19); no further descriptions were found in the literature. Results of goniometric measurement are listed in the following tables.

(a) Papaverine

Needle-shaped crystals, orthorhombic system, class 222.

Forms	φ	6		
110	72° 18'	90° 00′		
011	0° 00'	23° 11'		
100	90° 00′	90° 00'		
120	57° 33'	90° 00'		
010	0° 00'	90° 00'		
112	72° 18'	34° 45'		

Forms in order of development: 110, 011, 100, 120, 010, 112.

$$a:b:c = 0.3267:1:0.4252$$
.

Barker angles (Barker, 1930; Terpstra, 1946):

$$cr = 56^{\circ} 49', am = 33^{\circ} 27', bq = 32^{\circ} 27'.$$

The axial ratios, derived from the X-ray results, are:

$$a:b:c = 0.3175:1:0.2122.$$

The goniometric and X-ray settings are different. Transformation determinants for Groth's (G), Barker's (B) and the röntgenographic (R) settings are:

$R \rightarrow B$	002/200/010	$R \rightarrow G$	100/010/002
$B \rightarrow R$	010/002/100	$G \rightarrow R$	200/020/001
	$B \rightarrow G$	010/002/200	
	$G \rightarrow B$	001/200/010	

(b) Papaverine chlorhydrate

Prismatic crystals, monoclinic system, class 2/m.

Forms	arphi	ę		
110	50° 04'	90° 00′		
011	3° 31′	30° 32′		
121	32° 17′	54° 03′		
121	33 0° 22′	53° 23′		
<u>ī</u> 11	311° 19′	41° 29′		
111	51° 37′	43° 08'		
100	90° 00′	90° 00′		
$\overline{2}11$	293° 07'	56° 09′		
120	31° 08′	90° 00′		

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

$$a:b:c = 0.8370:1:0.5845$$
.

$$X_0' = 0.0367, \ \mu = 2^\circ \ 06', \ \beta = 92^\circ \ 06', \ d = 59^\circ \ 31', \ f = 53^\circ \ 43'.$$

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

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

(c) Papaverine bromhydrate

Isomorphous with papaverine chlorhydrate.

Forms	φ	Q		
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.

$$a:b:c = 0.8314:1:0.5789$$

$$X'_0 = 0.0405, \ \mu = 2^\circ 19', \ \beta = 92^\circ 19', \ d = 59^\circ 56', \ f = 53^\circ 36'.$$

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

Barker angles:

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

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

	$a({ m \AA})$	b (Å)	c (Å)	β	V (Å ³)	σ_c	Z
Papaverine	9.50	29.22	6 ∙35	·	1805	1.248	4
Papaverine. HCl	$13 \cdot 10$	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.

References

- BARKER, T. V. (1930). Systematic Crystallography. London: Murby.
- Beilsteins Handbuch der organischen Chemie (1935), 4th ed., vol. 21, p. 220. Berlin: Springer.
- GROTH, P. (1906–19). Chemische Krystallographie, vol. 5, p. 947. Leipzig: Engelmann.
- TERPSTRA, P. (1946). Kristallometrie. Groningen: Wolters.

Acta Cryst. (1953). 6, 665

A nomogram for evaluating the temperature factor.* By H. J. GRENVILLE-WELLS, Laboratory for Insulation Research, Massachusetts Institute of Technology, Cambridge, Massachusetts, U.S.A.

(Received 1 April 1953)

The nomogram evaluates the expression

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

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

$$f_{t} = f_{0} \exp \left[(-2B \sin^{2} \theta) / \lambda^{2} \right]$$
$$= f_{0} 10^{-\frac{2B}{\log_{\theta} 10} \cdot \frac{\sin^{2} \theta}{\lambda^{2}}} = f_{0} 10^{-\frac{B}{1 \cdot 15} \cdot \frac{\sin^{2} \theta}{\lambda^{2}}},$$

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 $B = 8\pi^2 \tilde{u}^2/3$ is found on the D scale, the line joining these points will cut the C scale at the point (B/1.15) $\times (\sin^2 \theta)/\lambda^2$. 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,

* Sponsored by the O.N.R., the Army Signal Corps and the Air Force under O.N.R. contracts N5ori-07801 and N5ori-07858.