$$\Delta\varrho = \varrho_o - \varrho_c\,,$$

and we have therefore obtained the shift, compensated for termination-of-series effects.

The slopes and curvatures may be computed either by direct summation at the given point from the relevant expressions, or else from a difference synthesis map. In the latter case it is customary to assume that the curvatures $\delta^2\varrho_c/\delta x^2$ are to all practical purposes equal to $\delta^2\varrho_o/\delta x^2$, and this statement holds in all cases (last-stage-refinement) where it is proposed to use it.

From the Gaussian shape of peak-density-distributions another helpful expression can be derived:

$$\varrho_r = Z.(p/\pi)^{3/2}.\exp(-pr^2)\,,$$

where p is a constant, Z the total number of electrons in the peak considered, and ϱ_r the electron density at a distance r from the summit. From this the compensated shift may now be written:

$$\Delta x = -(\delta\Delta\varrho/\delta x)/2p.\varrho_s\,.$$

Both p and the electron density of the summit, ϱ_s, can conveniently be derived from the F_o syntheses maps. It will not usually be necessary to know either value to a very high degree of precision since, in the polishing stages of refinement, slopes become small quantities and limited variations in the denominator of the given formula do not change Δx significantly.

When many atoms are involved in the refinement, as will be the case when a large molecule is found to be in general position, the evaluation of shifts by purely arithmetical means becomes a formidable undertaking and is hardly ever attempted without the aid of sophisticated machinery. The ΔF map is less unwieldy but even with careful contour plotting yields slope values of rather limited accuracy.

Another approach to this predicament (not in itself novel) was found to be practical since it involves only standard punched-card equipment for Beevers–Lipson summations.

The slope values are plotted as a function of the coordinates, and for the most general centrosymmetrical case, space group $P\bar{1}$, the slope in the x direction is given by the relation

$$\delta\Delta\varrho/\delta x = -(4\pi/aA).\Sigma\Sigma h.\Delta F.\sin(hx+ky)$$

in the abbreviated notation, where $\Delta F = F_o - F_c$. This expression can, of course, be expanded in the usual way to be handled by one-dimensional summation. Similar relations hold for the shifts in the direction of the other axes.

For a single projectional refinement two slope maps are therefore necessary. The input parameters for the atomic positions may be drawn in the slope maps, and the slope values at these points found by simple interpolation techniques. It was found that whereas the slopes, deduced from very carefully drawn difference maps, would vary within 15% of the numerically accurate values, the slopes found from slope maps would give only a 6% maximum discrepancy.

The necessity for curvature maps, analogous to the slope maps, will not as a rule arise, but they could of course be prepared in extreme cases; the same holds for the cross-term derivatives when the assumption of orthogonality and sphericity will not hold to a good approximation.

The refinement procedure outlined above was used for a carotenoid compound containing 43 atoms in general position, so as to obtain simultaneous compensated shifts. The ΔF difference map was used for a general assessment of scaling and temperature-factor adjustment in this stage. The method was found to be relatively fast and of satisfactory accuracy.

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Phase relations in the plagioclase felspars: composition range An_0 to An_{70}.

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(*Received* 16 *November* 1954)

This communication summarizes recent observations on materials covering nearly the whole plagioclase series.

(1) Cole, Sörum & Taylor (1951) observed no departure from the low-temperature albite-type structure in plagioclase samples containing up to about 30% An. The coexistence of two plagioclases in this composition range was first reported by Laves (1951), and later confirmed by one of us (J. V. S., in collaboration with Dr W. S. MacKenzie, Geophysical Laboratory, unpublished). Laves (1954) has concluded that 'low-temperature' plagioclases within the range An_5 to An_{17} consist of two phases.

We also have examined a number of specimens in the region An_0–An_{20} from low-temperature environments (both specimens showing schiller ('peristerites'; Böggild, 1924) and specimens devoid of schiller). In agreement with Laves we have found that all the specimens in the region An_5–An_{17} are unmixed. The lattice angles of the two phases agree closely with those found by Laves and the compositions deduced from the curves of lattice parameters determined by Smith (1954) are $An_{3\pm2}$ and $An_{23\pm2}$. The failure of previous workers, using powder methods, to detect this type of unmixing in albite-oligoclases is not surprising in view of the poor resolution of the powder method.

In spite of this evidence, which suggests that all low-temperature oligoclases are unmixed, some evidence (not regarded as conclusive) has been obtained by one of us (J. V. S., in collaboration with Dr W. S. MacKenzie, Geophysical Laboratory) which suggests that the two-phase region lies below the high–low inversion and that homogeneous crystals may exist in the low-temperature state. This point is under further examination.

(2) For the range An_{50}–An_{70}, further measurements have confirmed that the separation of the pairs of sub-

sidiary layer lines in *c*-axis photographs varies linearly with chemical composition, as stated by Cole *et al.* Further work in the region An_{20}–An_{50} shows that this intermediate type of structure extends at least to An_{23}, and that the separation of the pairs of subsidiary layer lines which characterize the structure varies linearly with chemical composition over the *whole* range. The subsidiary reflexions are sharp in the range An_{70}–An_{40} and then become progressively more diffuse as the An content decreases. Those observations will be discussed in detail elsewhere (Gay, 1954).

The new observations are in disagreement with the homogeneity found by Laves (1954) for specimens in the region An_{20}–An_{38}.

(3) All specimens in the region An_0–An_{90} may be homogenized into the high-temperature albite-type structure by prolonged heating at elevated temperatures. Homogeneous natural specimens of this kind may sometimes be found.

Further work is in progress to ascertain the relations between the two unmixing regions and the high–low inversion interval. Full details of the work on the intermediate plagioclases will be given shortly by Gay, and details of the work on the albite-oligoclases, together with the mineralogical implications, will be given later.

It is a pleasure to thank Dr W. H. Taylor for his continued advice and Dr W. S. MacKenzie for the information acknowledged in the text.

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Crystallographic properties of phenacaine hydrochloride monohydrate.

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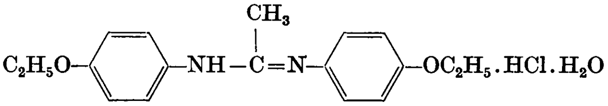
(*Received* 3 *August* 1954)

Phenacaine hydrochloride (holocaine hydrochloride), used medicinally as an ocular anesthetic, has the chemical name N^1–N^2–bis(*p*-ethoxyphenyl) acetamidine hydrochloride. A brief mention of the optical properties is made by Winchell (1943), but no X-ray data have appeared. The compound is represented by the structural formula:



Crystallization from water results in 010 blades elongated parallel to *c*. The sample used for this study lost water at about 95° C. and melted 192–5° C. The crystal system is monoclinic with space group C_2^2–$P2_1$ and two molecules per cell.

$$a = 8{\cdot}13,\ b = 23{\cdot}75,\ c = 5{\cdot}44\ \text{Å};\ \beta = 115^\circ\ .$$

The optical properties are:

$\alpha = 1{\cdot}520$, $\beta = 1{\cdot}600$; $(-)2V =$ about 80°. The optic plane is perpendicular to 010, $\alpha : a = 8^\circ$ in acute β. Winchell (1943) gives $\alpha = 1{\cdot}523$, $\beta = 1{\cdot}600$, $\gamma = 1{\cdot}74$, $(-)2V = 75^\circ$.

The powder data (Table 1) were obtained using a camera 114·6 mm. in diameter with chromium radiation and a vanadium pentoxide filter. A wavelength value of 2·2896 Å was used in the calculations.

Table 1. *X-ray powder diffraction data for phenacaine hydrochloride monohydrate*

d (Å)	I/I_1	*hkl*	*d* calculated from *a*, *b*, *c* and *β* (Å)
11·78	0·06	020	11·88
7·38	0·25	100	7·37
6·97	0·25	110	7·04
6·24	0·25	120	6·26
5·95	0·25	040	5·94
5·40	0·13	130	5·39
5·25	0·25	$10\bar{1}$	5·25
4·93	0·50	001	4·93
4·83	0·25	011	4·83
4·56	0·13	021	4·55
3·95	0·13	060	3·96
3·77	1·00	$21\bar{1}$	3·78
3·68	0·25	200	3·69
3·64	0·25	$22\bar{1}$	3·64
3·51	0·13	220	3·52
3·43	0·50	—	—
3·19	0·75	—	—
2·967	0·13	—	—
2·623	0·13	—	—
2·477	0·13	—	—
2·451	0·13	—	—

Reference

Winchell, A. N. (1943). *Optical Properties of Organic Compounds*, p. 121. Madison: University of Wisconsin Press.