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## Crystallographic data for certain alkaloids. III.

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The cell dimensions for these substances (Table 1) were obtained from oscillation and Weissenberg photographs using Cu $K\alpha$ radiation. Densities were determined by flotation. The maximum error in the numerical data given is of the order of 1%.

### Ephedrine, $C_{10}H_{15}NO \cdot \frac{1}{2}H_2O$

Ephedrine is reported to occur in two forms: one is anhydrous and the other contains half a molecule of water of crystallization. Attempts to prepare the anhydrous form were unsuccessful. Oscillation photographs of the hydrated form showed the crystals to be orthorhombic with Laue symmetry *mmm*. This, in conjunction with the systematic absences, determines the space group uniquely as $C222_1$. The results obtained are compared in Table 1 with those given by Gossner & Neff (1935).

### Hordenine sulphate, $(C_{10}H_{15}NO)_2 \cdot H_2SO_4 \cdot H_2O$

Crystals were obtained by recrystallization from methanol. Oscillation photographs showed that the crystals were monoclinic (Laue symmetry $2/m$). Systematic absences indicated an $a$ glide and a screw axis. The space group is therefore uniquely determined as $P2_1/a$. The monoclinic angle was measured from a Weissenberg photograph of the [010] zone of reflexions.

### Homatropine, $C_{16}H_{21}NO_3$

Crystals were obtained by recrystallization from ethanol. Oscillation photographs determined the space group uniquely as $P2_1/c$. The monoclinic angle was again measured from a Weissenberg photograph.

### Homatropine hydrobromide, $C_{16}H_{21}NO_3 \cdot HBr$

Crystals were obtained by recrystallization from water. Oscillation and Weissenberg photographs determined the space group uniquely as *Pcab*.

In both homatropine and homatropine hydrobromide the nitrogen atom may be optically active, in which case, since the space groups are centro-symmetric, the unit cells must be assumed to contain equal numbers of L- and D-molecules. The alkaloid homatropine is a synthetic product (Manske & Holmes, 1950) so that a racemate is probable.

### Physostigmine, $C_{15}H_{21}N_3O_2$

The crystals obtained by recrystallization from ethanol were in the form of plates. Oscillation photographs showed the Laue symmetry to be *mmm* and the only absences to be screw absences along each axis. The space group is therefore determined uniquely as $P2_12_12_1$.

### Narcotine, $C_{22}H_{27}NO_7$

Long needle-shaped crystals were obtained by recrystallization of the commercial product from ethanol. As in physostigmine, the Laue symmetry and systematic absences determine the space group uniquely as $P2_12_12_1$.

### Quinidine benzenate, $C_{20}H_{24}NO \cdot \frac{1}{4}C_6H_6$

Crystals were obtained from a solution of quinidine in benzene. The space group was determined uniquely from oscillation photographs as $P2_12_12_1$.

The formula given by Groth (1906–19) is

$$C_{20}H_{24}NO \cdot \tfrac{1}{3}C_6H_6 ,$$

but the density calculated from this formula and the observed cell edges did not agree with that observed. Also the axial ratios

$$a:b:c = 0{\cdot}735:1:1{\cdot}24$$

did not agree with those given by Groth ($a:b:c$ = 0·6916:1:1·0054).

When the formula $C_{20}H_{24}NO \cdot \frac{1}{4}C_6H_6$ was adopted, agreement was found between observed and calculated densities. It is concluded that the material examined differed from that used for the observations quoted by Groth.

No further X-ray work on these substances is contemplated.

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Table 1

| Compound | $a$ (Å) | $b$ (Å) | $c$ (Å) | $\beta$ (°) | Density (g.cm.$^{-3}$) Obs. | Calc. | $Z$ | Space group |
|---|---|---|---|---|---|---|---|---|
| Ephedrine | 7·41 | 11·40 | 24·1 | — | 1·12 | 1·13 | 8 | $C222_1$ |
| Ephedrine (Gossner & Neff) | 7·41 | 11·25 | 24·1 | — | 1·124 | 1·15 | 8 | $C222_1$ |
| Hordenine sulphate | 24·1 | 8·29 | 11·75 | 103 | 1·31 | 1·29 | 4 | $P2_1/a$ |
| Homatropine | 14·5 | 15·1 | 6·97 | 100 | 1·21 | 1·22 | 4 | $P2_1/c$ |
| Homatropine hydrobromide | 10·3 | 16·4 | 19·25 | — | 1·48 | 1·46 | 8 | *Pcab* |
| Physostigmine | 7·24 | 14·25 | 14·50 | — | 1·20 | 1·22 | 4 | $P2_12_12_1$ |
| Narcotine | 7·90 | 15·4 | 32·6 | — | 1·38 | 1·38 | 8 | $P2_12_12_1$ |
| Quinidine benzenate | 9·42 | 12·8 | 15·85 | — | 1·19 | 1·19 | 4 | $P2_12_12_1$ |