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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)	β (°)	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	$P2_12_12_1$