molecule has therefore the anticipated planar configuration. The molecular arrangement within a layer can be derived unambiguously from the approximately known dimensions of the molecule and the dimensions of the unit cell. Fig. 1 is a schematic drawing of one layer of molecules; the dimensions chosen for the amide group are similar to those found in glycyl asparagine, and the N · · · O vector of the hydrogen bond between identical molecules in adjacent unit cells is taken to form an angle of 120° with the C–N bond. It also is assumed that the molecule possesses a true center of symmetry, which is very probably correct, and thus the space group of the crystal is $C2/c$. In the resulting molecular arrangement each nitrogen atom forms two good hydrogen bonds.

The two equivalent layers of molecules at $x = \frac{1}{4}$ and $x = \frac{3}{4}$, respectively, which are related by a twofold axis at $x = \frac{1}{2}$, $z = \frac{1}{4}$, are displaced in respect to each other in such a way that the bulky methylene groups of the molecules in one layer fit into the gap between the amide groups of two identical molecules in the other layer; so the close approach of 3·40 Å between two layers is made possible.

The correctness of the proposed structure has been confirmed by a comparison between observed intensities and calculated structure factors of the (0*kl*) zone. For the refinement of the structure, it is intended to collect three-dimensional data by means of an X-ray spectrometer.

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Crystallographic data for certain alkaloids. II. Some miscellaneous alkaloids.

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The space groups, unit-cell dimensions and unit-cell contents of six alkaloids have been determined. The crystallographic data were obtained from oscillation and Weissenberg photographs while the densities were determined by flotation. A summary of these data is given in Table 1, and brief notes on the appearance of the specimens and the space-group determinations are given in the text. Powder data for all these substances are being added to the A.S.T.M. index.

Brucine, $C_{23}H_{26}N_2O_4 . 4H_2O$

Brucine was recrystallized from a mixture of ethanol and water as colourless needles, elongated along [100] and bounded by the forms {100}, {010} and {001}. The Laue symmetry is *mmm* and the systematic absences indicate uniquely the space group $P2_12_12_1$.

Brucine sulphate, $[C_{23}H_{26}N_2O_4]_2 . H_2SO_4 . 7H_2O$

This compound recrystallized from water as colourless laths elongated in the direction [100] and bounded by the forms {110}, {010} and {001}. The Laue symmetry is *mmm* and the systematically absent reflexions are (00*l*) when *l* is odd and (*hkl*) when $h+k$ is odd. These characterize uniquely the space group $C222_1$. The number of formula units per unit cell, calculated from unit-cell dimensions and the observed density, is four; consequently each sulphate ion must lie on a diad axis. The seven molecules of water are possibly arranged in a manner similar to that of the molecules of water in the structure of strychnine sulphate pentahydrate (Bokhoven, Schoone & Bijvoet, 1951).

Gelsemine hydrochloride, $C_{20}H_{22}N_2O_2 . HCl$

This compound was recrystallized from water as very small transparent laths. The Laue symmetry, *mmm*, and the systematic absences show that the space group is $P2_12_12_1$.

α-Lobeline hydrochloride, $C_{22}H_{27}NO_2 . HCl . H_2O$

α-Lobeline hydrochloride recrystallized from water as transparent needles. The space group of this substance, as indicated by the Laue symmetry and systematic absences, is $P2_12_12_1$. Calculation of the unit-cell contents from the cell dimensions and the observed density requires a molecule of water to be associated with each formula unit.

Pilocarpine hydrochloride, $C_{11}H_{16}N_2O_2 . HCl$

Commercial specimens were used in the investigation of this compound. The Laue symmetry is $2/m$ and the reflexions (0*k*0) are systematically absent when *k* is odd. This is indicative of the space groups $P2_1$ and $P2_1/m$, but as the compound is optically active the space group must be the non-centrosymmetric one, $P2_1$.

Pilocarpine hydrobromide, $C_{11}H_{16}N_2O_2 . HBr$

Crystals of two habits were obtained from a solution of pilocarpine in aqueous hydrobromic acid. One habit

Table 1. *Crystallographic data*

Compound	Space group	a (Å)	b (Å)	c (Å)	β	Density (g.cm.$^{-3}$) Obs.	Density (g.cm.$^{-3}$) Calc.	No. of formula units/unit cell
Brucine	$P2_12_12_1$	7·6	11·6	26·6	—	1·31	1·32	4
Brucine sulphate	$C222_1$	12·3	14·4	26·9	—	1·41	1·41	4
Gelsemine hydrochloride	$P2_12_12_1$	7·3	9·0	26·4	—	1·37	1·37	4
α-Lobeline hydrochloride	$P2_12_12_1$	8·1	14·2	18·0	—	1·24	1·25	4
Pilocarpine hydrochloride	$P2_1$	6·7	9·2	10·8	105½°	1·26	1·26	2
Pilocarpine hydrobromide	$P4_1$	6·9	6·9	37·6	—	2·12	2·11	8

consisted of long tapering needles; the other of square plates. The latter when viewed in convergent plane-polarized light shows a uniaxial brush. Crystals of both habits are reddish-brown in colour and give identical X-ray diffraction patterns. The Laue symmetry is $4/m$ and the reflexions $(00l)$ are absent when l is not a multiple of 4. The possible space groups are $P4_1$ and $P4_1/m$, but as the base from which the compound was prepared is optically active the space group must be $P4_1$. Up to the present time it has not proved possible to obtain the hydrobromide in a form isomorphous with the hydrochloride.

A detailed investigation of the structure of pilocarpine hydrochloride is in progress and similar investigations are to be started in the near future of α-lobeline hydrochloride and gelsemine hydrochloride.

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Sayre's equation and Zachariasen's method.

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A recent note by Krogh-Moe (1953) provides a derivation, in a modified form, of an equality relation between structure factors first obtained by Sayre (1952). The new derivation is of interest in that Krogh-Moe appears to obtain his equation (12) (referred to here as (12–K.-M.)) without imposing Sayre's condition of equal atoms. The purpose of the present note is to point out that (12–K.-M.) is valid only in the equal-atom case, and that Zachariasen's (1952) equation (11–Z.) is also not generally valid. The derivation of this equation, on which Zachariasen's method is based, has already been criticised by Lavine (1952).

We define a unitary structure factor

$$U(\mathbf{h}) = 2\sum_{j=1}^{\frac{1}{2}N} n_j \cos 2\pi\mathbf{h}.\mathbf{r}_j\,. \tag{1}$$

There is a corresponding distribution in crystal space

$$\sigma(\mathbf{r}) = \frac{1}{V}\sum_{h<H} U(\mathbf{h}) \cos 2\pi\mathbf{h}.\mathbf{r}\,. \tag{2}$$

If we now put

$$\sigma^2(\mathbf{r}) = \frac{1}{V}\sum_{h<2H} G(\mathbf{h}) \cos 2\pi\mathbf{h}.\mathbf{r} \tag{3}$$

it may readily be shown (see, e.g. Sayre, 1952) that

$$G(\mathbf{h}) = \frac{1}{V}\sum_{h'<H} U(\mathbf{h}')U(\mathbf{h}-\mathbf{h}')\,. \tag{4}$$

Equation (4) is true in all circumstances. If, however, the limits of the Fourier series (2) are set sufficiently high for the 'atoms' of $\sigma(\mathbf{r})$ to be completely resolved from one another, those of $\sigma^2(\mathbf{r})$ are also resolved and corresponding to

$$\left.\begin{array}{lr} U(\mathbf{h}) = 2\sum_{j=1}^{\frac{1}{2}N} n_j \cos 2\pi\mathbf{h}.\mathbf{r}_j & (1) \\ \text{we have} & \\ G(\mathbf{h}) = 2\sum_{j=1}^{\frac{1}{2}N} g_j(h) \cos 2\pi\mathbf{h}.\mathbf{r}\;. & \end{array}\right\} \quad (5)$$

Each g_j is proportional to n_j^2.