sluggish, requiring several days' heating, but the crystals did not shatter. X-ray photographs of the products showed that both transformations gave rise to a random array of small crystallites which were either produced directly by breaking-up of the larger original crystal or by a complete disintegration of the original structure, followed by recrystallization. In either case the experiments do not demonstrate any structural resemblance between the two modifications which could be used to elucidate one of the crystal structures with the help of the other.

We wish to thank Prof. J. D. Bernal, F.R.S., for his interest, and the Building Research Station for assistance with experimental work. The work was carried out as part of an extra-mural contract for the Building Research Board and we thank the Director of Building Research for permission to publish this paper.

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Acta Cryst. (1953). **6**, 808

The crystal structure of succinamide, $(CH_2CONH_2)_2$.*

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(*Received* 15 *June* 1953)

A considerable amount of accurate information has been collected about the configuration and dimensions of the peptide amide group, whereas comparable data for the terminal amide group are still missing. Only three crystal structure determinations of compounds containing the terminal amide group have been published, namely, those of acetamide (Senti & Harker, 1940), L-glutamine (Cochran & Penfold, 1952) and glycyl-L-asparagine (Pasternak, Katz & Corey, 1954; see also Katz, Pasternak & Corey, 1952); the dimensions reported for the group are appreciably different. For this reason an accurate crystal structure analysis of a simple amide would be of interest. The crystals of succinamide appeared to be specially suitable for a study, because of the simple molecular structure of this compound and also because a planar configuration was expected for its molecule by analogy to related compounds. In crystals of succinic acid the molecule is extended and planar (MacGillavry, Hoogschagen & Sixma, 1948; Morrison & Robertson, 1949), and the same holds for the succinamic acid part of glycyl-L-asparagine. If the molecule of succinamide also is extended and planar, then each of the two C–N bonds and the central C–C bond have to be *trans* for steric reasons, and the molecule has, like the molecule of succinic acid, a center of symmetry.

Crystals of succinamide (decomposition point about 250° C.) were easily obtained from water in monoclinic plates bounded by (001) faces. Perfect cleavage along (100) indicated a layer structure parallel to this plane. The unit-cell dimensions derived from rotation and Weissenberg photographs are

$$a_0 = 6{\cdot}96,\ b_0 = 8{\cdot}02,\ c_0 = 9{\cdot}90\ \text{Å},\ \beta = 102{\cdot}5°;$$

density (by flotation) = 1·442 g.cm.$^{-3}$; number of molecules $n = 4$ (calc. 3·98); systematic absences, hkl when $h+k$ is odd, $h0l$ when h and l are odd. These absences are characteristic for the space groups Cc ($n = 4$) and $C2/c$ ($n = 8$). Since there are only four molecules in the unit cell, this latter centrosymmetric space group would require the molecule to lie on a center of symmetry.

In addition to the systematic absences, very pronounced pseudo-absences are observed in the ($hk0$) zone; reflections with h and k both odd are missing except two which are extremely weak. By contrast, the ($h00$) reflections are outstandingly strong and show the normal decline. This intensity pattern is compatible only with a layer structure parallel to (100) with all the atoms lying almost exactly in the planes $x = \frac{1}{4}$ and $x = \frac{3}{4}$; the

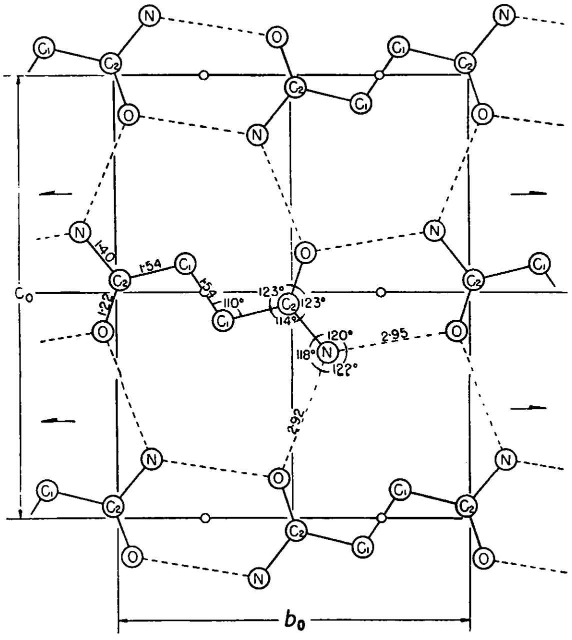

Fig. 1. The arrangement of the molecules of succinamide within the layer $x = \frac{1}{4}$ or $x = \frac{3}{4}$.

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* Contribution No. 1819 from the Gates and Crellin Laboratories. This investigation was supported in part by a research grant, RG-1987, from the National Institute of Health, Public Health Service.

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 $\cdots$ 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 $(0kl)$ 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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Acta Cryst. (1953). **6**, 809

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

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(*Received* 24 *July* 1953)

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 $(00l)$ 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 $(0k0)$ 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