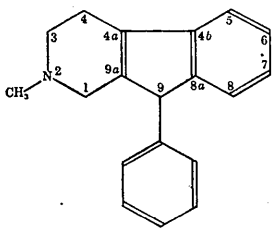
(1) and (2) and other derivatives with the ring system (I) are biologically active, whilst (4) is nearly inactive.

X-ray data

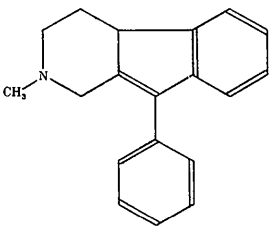
X-ray single-crystal photographs were taken, and the density was determined in a mixture of CCl_4 and C_6H_6. The results of the measurements are:

Compound	Space group	a (A.)	b (A.)	c (A.)	β (°)	Density (g.cm.$^{-3}$)
(1) Thephorin	$P2_1/c$	5·53	9·37	31·2	115	1·17
(2) Thiocyanate	$P2_1/n$	10·68	10·74	14·80	100	1·27
(3) Dihydroxy	$P2_1/c$	12·85	8·30	14·64	99	1·26
(4) Nitrate	Aa	8·24	10·94	18·58	92	1·28

The compounds all have four molecules per unit cell (calculated 3·96–3·99).



I



II

Thephorin

Morphology and optics

Each compound was examined under the polarizing microscope with the following result:

(1) *Thephorin*

Small, monoclinic needles elongated along [100], bounded by {001} and {011}.

$\beta \parallel b$; γ about 5° from c. Negative. Optic axial angle medium.

(2) *Thephorin thiocyanate*

Monoclinic prisms elongated parallel to [010]. Forms {001}, {101} and {10$\bar{1}$} developed, the last one predominant.

$\beta \parallel b$; α and γ approximately parallel to a and c respectively. Positive. $2E \simeq 80°$.

(3) *Dihydroxy-dihydro-thephorin*

Well-developed monoclinic prisms, elongated along [010], bounded by {100}, {001} and {10$\bar{2}$}.

$\alpha \parallel b$; γ lies about 25° from c in the acute angle. Negative. $2V \simeq 70°$.

(4) *Nitrate of isomeric thephorin*

The crystals occur either as nearly hexagonal prisms elongated along a, or in a scalenohedral-like habit.

$\gamma \parallel b$; α lies 20° from a in the obtuse angle. Negative. Optic axial angle very small.

Discussion

In thephorin the birefringence is negative, the α-vibration direction is nearly perpendicular to the a plane, the a axis is short, and the 100 reflexion is strong. This suggests that the molecules are lying approximately parallel to the a plane.

The nitrate derivative is interesting crystallographically, as it has strongly pseudohexagonal symmetry. This is shown by the X-ray diffraction pattern on the 0*kl* zone, as well as by the optical and morphological properties, which are nearly those of a uniaxial crystal.

A model of the main ring-systems (I and II) based on the chemically established formulae and accepted bond distances can be represented roughly by a very flat trigonal prism with sides about 9A. This general shape and size of the molecules is confirmed by the investigation. Thephorin shows that the three six-membered rings in the molecule cannot be much tilted in relation to each other, and the hexagonal character of the nitrate derivative is probably related to the apparent threefold symmetry of the molecules.

However, the differences in biological activity between these closely related compounds appear to be linked with differences in stereochemical *detail*. A complete X-ray analysis of one or more of the substances is therefore needed before an attempt can be made to correlate physiological activity with stereochemical configuration. Crystallographically thephorin suggests itself for this purpose.

Reference

LEHMANN, G. (1948). *J. Pharmacol.* **92**, 249.

Notes and News

Announcements and other items of crystallographic interest will be published under this heading at the discretion of the Editorial Board. Copy should be sent direct to the British Co-editor (R. C. Evans, Crystallographic Laboratory, Cavendish Laboratory, Cambridge, England).

International Union of Crystallography

Further formal notification of adhesion has been given, as follows:

On 14 December 1948 by the Netherlands.

On 15 December 1948 by Australia through the Australian National Research Council.

On 23 December 1948 by France through the Académie des Sciences de l'Institut de France.