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Crystallographic data of promazine and chlorpromazine.

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Promazine, $C_{17}H_{20}N_2S$, is orthorhombic with $a=18{\cdot}54\pm3$, $b=20{\cdot}39\pm3$, $c=8{\cdot}22\pm2$ Å, $V=3107$ Å^3 (space group *Pmnb* or *Pbn*2_1). Chlorpromazine, $C_{17}H_{19}ClN_2S$, is orthorhombic with $a=15{\cdot}20\pm3$, $b=23{\cdot}53\pm3$, $c=9{\cdot}27\pm2$ Å, $V=3315$ Å^3 (space group *Pbca*).

As part of a crystallographic investigation of substances affecting the nervous system, some heavy tranquillizers and their chemical relatives have been studied. The X-ray and optical properties of promazine [10-(3-dimethylaminopropyl)phenothiazine] and chlorpromazine [10-(3-dimethylaminopropyl)-2-chlorophenothiazine] are presented.

Promazine

Promazine, $C_{17}H_{20}N_2S$, provided by May and Baker, England, was recrystallized slowly from ether at about 4°C. It formed elongated plates, the habit of which can be seen in Fig. 1(*a*) in relation to the principal optic directions and the chosen crystallographic axes.

Optical: Biaxial positive

$\gamma=1{\cdot}78\pm1$
$\beta=1{\cdot}642\pm3$
$\alpha=1{\cdot}629\pm3$
$2V_{obs}=41{\cdot}8°\pm1{\cdot}0°$
$2V_{calc}=36{\cdot}4°\pm6{\cdot}8°$
$B=0{\cdot}15$

Weissenberg and rotation photographs taken with Cu $K\alpha$ radiation revealed that the unit cell was orthorhombic. The systematic absences were $hk0$ when k was odd and $h0l$ when $h+l$ was odd. This indicates the space group either *Pmnb* or *Pbn*2_1.

The unit-cell dimensions are

$a=18{\cdot}54\pm3$ Å
$b=20{\cdot}39\pm3$
$c=8{\cdot}22\pm2$
$V=3107$ Å^3

The observed and the calculated densities of 1·214 and 1·215 g.cm^{-3}, assuming 8 molecules with a molecular weight of 284·42, are in good agreement. Thus the space group *Pmnb* having 8 general positions seems more probable than *Pbn*2_1 which would require 2 molecules in the asymmetric unit.

Chlorpromazine

A sample of chlorpromazine, $C_{17}H_{19}ClN_2S$, provided by AB Leo, Sweden, was recrystallized from ethanol at about −2°C. The habit of the crystal plates formed can be seen in Fig. 1(*b*) where the principal optic directions in relation to the crystallographic axes also are shown.

Optical: Biaxial positive

$\gamma=1{\cdot}77\pm1$
$\beta=1{\cdot}665\pm3$
$\alpha=1{\cdot}595\pm3$
$2V_{obs}=83°\pm1°$
$2V_{calc}=82{\cdot}8°\pm4{\cdot}8°$
$B=0{\cdot}18$

Weissenberg and rotation photographs were taken with Cu $K\alpha$ radiation. These showed that the unit cell was orthorhombic with the following systematic absences: $0kl$ for l odd, $h0l$ for h odd and $hk0$ for k odd. This indicates space group *Pbca*.

The unit-cell dimensions are

$a=15{\cdot}20\pm3$ Å
$b=23{\cdot}53\pm3$
$c=9{\cdot}27\pm2$
$V=3315$ Å^3

The observed density was 1·274 g.cm^{-3}, which corresponds well to the calculated value 1·277, assuming a molecular weight of 318·86 and $Z=8$. The unit cell and space group data are in good agreement with the values found by Feil, Linck & McDowell (1965).

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References

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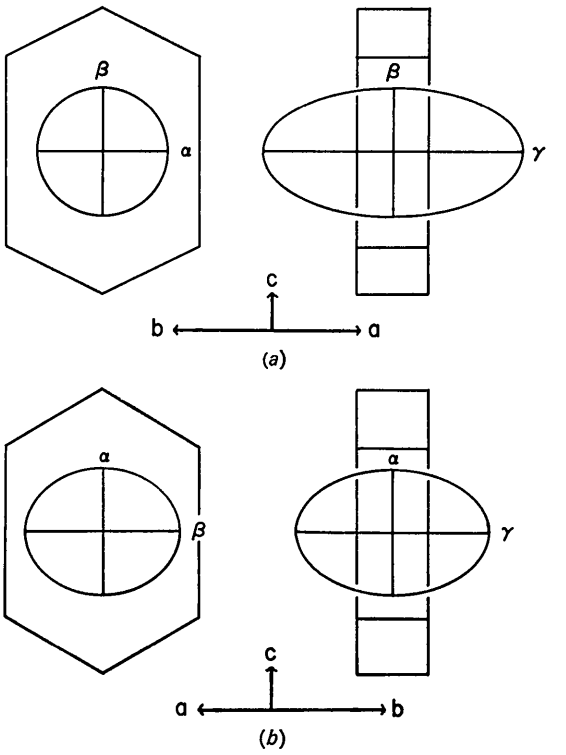

Fig. 1. Common crystal habit, the indicatrix and chosen crystallographic axes of (*a*) promazine and (*b*) chlorpromazine. The differences between the principal optic axes are exaggerated while the lengths of the arrows are proportional to the respective crystallographic axes.