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Bicuculline and narcotine: preliminary structure data.

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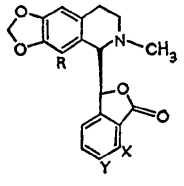
The alkaloids bicuculline and narcotine form crystals with space group $P2_12_12_1$. The cell dimensions are, respectively, $a=10{\cdot}916$, $b=14{\cdot}478$, $c=10{\cdot}447$ Å, and $a=15{\cdot}398$, $b=32{\cdot}686$, $c=8{\cdot}022$ Å. Other preliminary data are listed.

Bicuculline, $C_{20}H_{17}NO_6$, a phthalideisoquinoline alkaloid, is of current interest due to its possible activity as a specific antagonist of the inhibitory function of γ-aminobutyric acid in the mammalian central nervous system (Curtis, Duggan, Felix & Johnston, 1970; Steward, Player, Quilliam, Brown & Pringle, 1971). Preliminary structural data have been collected for this alkaloid and for a related phthalideisoquinoline alkaloid narcotine, $C_{22}H_{23}NO_7$. Less accurate data for narcotine have previously been reported by Lovell (1953).

Small prismatic crystals of bicuculline were obtained from ethanol/chloroform solution and larger needle crystals of narcotine from methanol.



Bicuculline
R=H
X,Y= $-OCH_2O-$

Narcotine
R=X=Y=OCH_3

Weissenberg photographs taken with Cu $K\alpha$ (1·5418 Å) radiation revealed the same systematic absences for both compounds:

$$h00,\ h=2n+1$$
$$0k0,\ k=2n+1$$
$$00l,\ l=2n+1,$$

defining unambiguously the space group $P2_12_12_1$. Cell dimensions were obtained from 2θ values of 44 reflexions from bicuculline and 32 reflexions from narcotine, using two axes in each case, measured with a counter diffractometer.

	Bicuculline	Narcotine
M.W.	367·34	413·41
m.p.(°C)	201	178
Crystal system	Orthorhombic	Orthorhombic
Space group	$P2_12_12_1$	$P2_12_12_1$
Cell Dimensions (Å) a	10·916 (6)	15·398 (12)
Cell Dimensions (Å) b	14·478 (12)	32·686 (36)
Cell Dimensions (Å) c (prism)	10·447 (5)	8·022 (8)
V(Å^3)	1651 (3)	4037 (11)
Z	4	8
ϱ_{calc}(g.cm^{-3})	1·478	1·360
ϱ_{exp}(g.cm^{-3})	1·49	1·38

Further crystallographic studies of these two alkaloids are not contemplated.

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The refinement of the structure of hexabromoethane.

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The structure of hexabromoethane (C_2Br_6) reported earlier has been confirmed and refined with a new set of three-dimensional data collected at 22° on an automated diffractometer with Cu $K\alpha$ radiation by the 2θ scan technique. The lattice parameters $a=12{\cdot}043\pm0{\cdot}002$, $b=10{\cdot}674\pm0{\cdot}002$, and $c=6{\cdot}705\pm0{\cdot}001$ Å were within one standard deviation of those previously reported. The measured density is 3·823 g.cm^{-3}, and, with $Z=4$, the calculated density is 3·88 g.cm^{-3}. The final R value is 6·4%. The average carbon–bromine distance is 1·944 with a bond scatter of 0·005 Å. Intramolecular distances are 3·15 Å for the two bromine atoms bonded to the same carbon atom and 3·42 Å for bromine atoms bonded to different carbon atoms. The shortest intermolecular distance is a 3·76 Å bromine–bromine contact. The average bond angle at a carbon atom is $109{\cdot}6\pm0{\cdot}9°$.

Introduction

The crystal structure of hexabromoethane was first reported by Snaauw & Wiebenga (1942); the space group and lattice constants had previously been reported by Yardley (1928). Since this structure contains the crystallographically unusual feature of a molecular center of symmetry which is non-coincident with a crystallographic center of sym-