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Preliminary X-ray crystallographic study of some psychoactive indole bases.

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Crystallographic data are given for the *N,N*-dimethyl, 5-hydroxy-*N,N*-dimethyl, 5-methoxy-*N,N*-dimethyl and 5-methoxy-*N*-methyl derivatives of tryptamine.

As part of a crystallographic investigation of substances affecting the central nervous system, some psychoactive indole bases have been studied: *N,N*-dimethyltryptamine (DMT), 5-hydroxy-*N,N*-dimethyltryptamine (5-OH-DMT or bufotenine), 5-methoxy-*N,N*-dimethyltryptamine (5-MeO-DMT) and 5-methoxy-*N*-monomethyltryptamine (5-MeO-MMT).

The X-ray data were obtained from oscillation and Weissenberg photographs with Cu $K\alpha$ radiation, except for DMT, the constants of which were determined with an automatic diffractometer, PAILRED, using Mo $K\alpha$ radiation.

The determinations of density were made by flotation in Clerici solution. The melting-points were measured in a Leitz hot-stage microscope.

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Table 1. *Crystallographic data of N,N-dimethyltryptamine(DMT), 5-hydroxy-N,N-dimethyltryptamine(5-OH-DMT or bufotenine), 5-methoxy-N,N-dimethyltryptamine(5-MeO-DMT) and 5-methoxymonomethyltryptamine(5-MeO-MMT)*

	DMT	5-OH-DMT	5-MeO-DMT	5-MeO-MMT
Empirical formula	$C_{12}H_{16}N_2$	$C_{12}H_{16}N_2O$	$C_{13}H_{18}N_2O$	$C_{12}H_{16}N_2O$
Molecular weight	188·26	204·27	218·30	204·27
Melting point	58·2°C	146·5°C	68·0°C	101·7°C
Crystal habit	Transparent acicular	Transparent prism	Transparent prism	Transparent prism
Crystal system	Monoclinic	Monoclinic	Monoclinic	Orthorhombic
Systematic absences	$0k0$ when k is odd $h0l$ when h is odd	$0k0$ when k is odd $h0l$ when h is odd	$0k0$ when k is odd	$00l$ when l is odd
Space group	$P2_1/a$	$P2_1/a$	$P2_1$ or $P2_1/m$	$P222_1$
Molecules per unit cell	$Z=4$	$Z=8$*	$Z=8$*	$Z=4$
Unit-cell dimensions	$a=$ 7·88±1 Å $b=$ 19·68±4 $c=$ 7·44±1 $\beta=$ 97·9° $V=1153{\cdot}8$ Å^3	$a=$ 18·11±2 Å $b=$ 11·56±3 $c=$ 14·53±3 $\beta=$ 131·5° $V=2277{\cdot}6$ Å^3	$a=$ 17·46±4 Å $b=$ 12·02±2 $c=$ 13·00±2 $\beta=$ 108·9° $V=2583{\cdot}4$ Å^3	$a=$ 11·56±4 Å $b=$ 12·44±3 $c=$ 7·96±5 $V=1144{\cdot}7$ Å^3
Density (observed)	1·096 g.cm^{-3}	1·205 g.cm^{-3}	1·123 g.cm^{-3}	1·196 g.cm^{-3}
Density (calculated)	1·088 g.cm^{-3}	1·191 g.cm^{-3}	1·122 g.cm^{-3}	1·182 g.cm^{-3}

* 5-OH-DMT and 5-MeO-DMT are dimers according to the Z values.

Notes and News

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Journal of Applied Crystallography

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