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Preliminary X-ray crystallographic study of some psychoactive indole bases. By ROLF BERGIN, DIEGO CARLSTRÖM, GÖRAN FALKENBERG and HANS RINGERTZ, *Department of Medical Physics, Karolinska Institutet, Stockholm 60, Sweden*

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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 ₂ O	C ₁₃ H ₁₈ N ₂ O	C ₁₂ H ₁₆ N ₂ O
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 β = 97.9° V = 1153.8 Å ³	a = 18.11 ± 2 Å b = 11.56 ± 3 c = 14.53 ± 3 β = 131.5° V = 2277.6 Å ³	a = 17.46 ± 4 Å b = 12.02 ± 2 c = 13.00 ± 2 β = 108.9° V = 2583.4 Å ³	a = 11.56 ± 4 Å b = 12.44 ± 3 c = 7.96 ± 5 V = 1144.7 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

Announcements and other items of crystallographic interest will be published under this heading at the discretion of the Editorial Board. The notes (in duplicate) should be sent to the General Secretary of the International Union of Crystallography (G. Boom, Laboratorium voor Technische Natuurkunde der Rijksuniversiteit, Westersingel 34, Groningen, The Netherlands). Publication of an item in a particular issue cannot be guaranteed unless the draft is received 8 weeks before the date of publication.

Journal of Applied Crystallography

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