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The Crystal and Molecular Structure of Bufotenine, 5-Hydroxy-(*N*,*N*)-dimethyltryptamine

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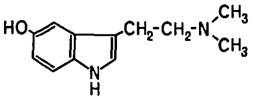
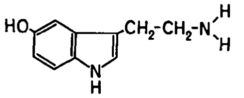
Bufotenine, or 5-hydroxy-(*N*,*N*)-dimethyltryptamine, crystallizes as a base in the monoclinic space group $P2_1/a$ with $a=17{\cdot}95$, $b=11{\cdot}52$, $c=14{\cdot}24$ Å; $\beta=131{\cdot}29°$; $Z=8$. Data were collected on a PAILRED automatic linear diffractometer. The structure was determined by the symbolic addition procedure and refined by the method of full-matrix least-squares to $R=0{\cdot}054$ for 1748 observed reflexions. The molecular structures of the two molecules in the asymmetric unit are almost identical. The indole nucleus of the *A*-molecule is planar; in the *B*-molecule there is a small angle of 1·5° between the pyrrole and benzene portions of the ring system. The ethylamine chain is almost fully extended, and lies approximately in a plane which is nearly perpendicular to the indole nucleus. This conformation is defined by the torsion angles τ_1, which is 87 and 72° for molecules *A* and *B* respectively, and τ_2 (175 and 170°). There are normal O-H···N hydrogen bonds linking the *A*-molecules (2·68 Å) and the *B*-molecules (2·72 Å) separately in two similarly arranged hydrogen-bonding systems.

Introduction

Bufotenine, or 5-hydroxy-(*N*,*N*)-dimethyltryptamine, is an indolealkylamine with a somewhat controversial pharmacology regarding its effects on the central nervous system. It was first isolated from toad venom, hence its name, and studied for its circulatory effects (Handovsky, 1920). Stromberg (1954) found bufotenine in seeds of *Piptadenia peregrina*, which were used by South American Indians for intoxicating purposes. Since then, it has been isolated from several hallucinogenic drugs of plant origin. Bufotenine was reported to be psychoactive in humans after intravenous injection (Hawkins & Fabing, 1956) but these results were not confirmed by further studies (Turner & Merlis, 1959). Later, bufotenine was claimed to occur in blood and urine of both normal and schizophrenic patients. The occurrence of bufotenine is of great interest, and Brune & Himwich (1962) suggested that it might be the psychotomimetic substance active in schizophrenia. The recent discovery of an enzyme, indolealkylamine-*N*-methyltransferase, in the human brain (Mandell & Morgan, 1971), shows that methylated indole derivatives really can be produced in the central nervous system. The differences in receptor activity between these compounds and serotonin may be due to steric factors, and an X-ray crystallographic study of bufotenine was undertaken accordingly.



Bufotenine



Serotonin

Experimental

Bufotenine base was kindly supplied by Professor Bo Holmstedt, Department of Toxicology, Karolinska

Institutet, Stockholm. Among the lens-shaped crystals several were large enough for single-crystal analysis. The crystal selected was colourless, transparent and highly birefringent and had, after trimming, the dimensions 0·3 × 0·3 × 0·4 mm. The long side of the rectangular cross section corresponded to the unique axis of the monoclinic space group found in the preliminary crystallographic study using Weissenberg techniques (Bergin, Carlström, Falkenberg & Ringertz, 1968). The crystal was mounted on a glass fibre with the unique axis *b* parallel to the ω axis of the automatic linear single-crystal diffractometer PAILRED (Philips), which was equipped with a graphite monochromator. The unit-cell parameters were measured at room temperature (20 ± 1 °C) using Mo $K\alpha$ radiation ($\lambda = 0{\cdot}7107$ Å). The density was measured by flotation in Clerici solution at 22·5 °C. The melting point was determined in a hot-stage microscope.

Crystallographic data for bufotenine

Empirical formula	$C_{12}H_{16}N_2O$
Molecular weight	207·27
Melting point	146·5 °C
Crystals	Transparent, colourless prisms
Crystal system	Monoclinic
Systematic absences	*h*0*l* when *h* is odd
	0*k*0 when *k* is odd
Space group	$P2_1/a$
Molecules per unit cell	$Z = 8$
Unit-cell dimensions	$a = 17{\cdot}95 \pm 0{\cdot}01$ Å
	$b = 11{\cdot}52 \pm 0{\cdot}01$
	$c = 14{\cdot}24 \pm 0{\cdot}02$
	$\beta = 131{\cdot}29 \pm 0{\cdot}03°$
	$V = 2220{\cdot}39$ Å^3
Density	$D_m = 1{\cdot}205$ g.cm^{-3}
	$D_x = 1{\cdot}191$ g.cm^{-3}

The intensities of the reflexions on the layers *h*0*l* through *h*12*l* were collected for $\sin\theta/\lambda \leq 0{\cdot}56$. In order to approximate to a fixed-count strategy, the fainter reflexions were scanned up to three times. The background intensity was measured for 0·4 min on each side of every reflexion. The continuous ω-scan had a scanning range of 4–5° and a scanning rate of 2·5° per min. In all, 3362 independent reflexions were recorded. Of these, 1602 (48 %) were not significantly different from the background level at a 95 % confidence limit and were considered as unobserved. Corrections were made for background, for Lorentz and polarization factors but not for absorption, owing to the low μ value (0·84 cm^{-1}). The corrected structure amplitudes were placed on an approximately absolute scale by Wilson statistics.

An X-ray crystallographic program system developed at the Department of Medical Physics by Bergin (1971) was used for all the calculations, which were carried out on an IBM 360/75 computer.

Determination of the structure

300 *E* values with $E \geq 1{\cdot}85$ were used for the phase determination, which was performed by generating solutions for the triple relations between phases (Karle & Karle, 1963, 1966). Using the indices of the reflexions, 1439 triple products were obtained ($|E_1 . E_2 . E_3| \geq 12{\cdot}0$). Three linearly independent reflexions were selected to specify the origin, and in addition, three other reflexions were given symbols. The basic set for applying the Sayre procedure (Sayre, 1952) consisted of:

Sign	*h*	*k*	*l*	$\vert E\vert$	Number of relations	Range for $P+$
+	−3	9	6	4·297	52	0·951–1·000
+	−1	8	6	4·238	63	0·940–1·000
+	1	9	5	3·877	41	0·939–1·000
a	−17	8	7	4·844	42	0·961–1·000
b	−20	0	14	4·419	34	0·945–1·000
c	−4	1	3	3·263	61	0·902–0·988

The Sayre relations were used to accumulate phases expressed in terms of the phases of the basic set by using an automatic procedure in the program system. Once the symbols had been assigned, 296 phases were obtained.

In a three-dimensional *E* map, 26 non-hydrogen atoms were located among the 40 strongest peaks. An additional Fourier synthesis with phases based on these 26 atomic positions revealed the four missing atoms and completed the determination of the non-hydrogen atoms of the two bufotenine molecules in the asymmetric unit.

Refinement of the structure

A full-matrix least-squares refinement of the positional parameters of the 30 atoms given isotropic temperature factors yielded an *R* value of 0·144 ($R = \sum||F_o| - |F_c|| / \sum|F_o|$). From a difference Fourier synthesis, 17 hydrogen atoms could be identified among the 32 strongest maxima. With anisotropic temperature factors for the non-hydrogen atoms and with hydrogen atoms introduced at the positions indicated by the difference maps, the *R* value dropped to 0·094 after three cycles of refinement. A difference Fourier synthesis prepared at this stage revealed the positions of the missing 15 hydrogen atoms. On inspection of the observed structure amplitudes, it was found that the strongest reflexions were impaired by extinction and the seven highest F_o were hence excluded from further calculations. Two cycles of refinement of the non-hydrogen atoms gave an *R* value of 0·055. After two additional refinement cycles of the hydrogen positions the *R* value decreased to 0·054. The last two cycles produced a better ratio between the estimated standard deviations and the shifts of the parameters. The last shifts for all atoms were less than 0·5 of the corre-

Table 1. *Observed and calculated structure factors*

The five columns in each group represent *h*, *k*, *l*, |*F*o|, *F*c.

0	0	2	79.4	-80.0
0	0	3	12.2	12.7
0	0	4	9.6	-8.3
0	0	5	11.1	13.4
0	0	8	32.9	-31.4
0	0	9	10.2	13.5
0	0	10	6.7	13.0
0	0	12	7.3	9.3
0	1	3	12.0	-13.0
0	1	4	18.1	16.7
0	1	8	8.3	-8.2
0	1	9	17.3	-17.2
0	1	10	12.8	13.6
0	1	11	12.4	14.0
0	2	2	21.1	-21.2
0	2	3	6.5	5.8
0	2	4	43.0	42.4
0	2	6	42.6	-41.5
0	2	7	13.9	13.1
0	2	8	10.6	-10.6
0	2	11	11.5	-12.9
0	3	2	8.0	-8.8
0	3	3	19.6	-19.7
0	3	4	15.4	-15.5
0	3	5	35.0	-32.8
0	3	6	15.9	15.0
0	3	7	6.4	7.2
0	3	8	6.3	6.4
0	3	10	7.9	-8.9
0	4	2	29.3	-30.3
0	4	3	32.2	31.2
0	4	4	15.0	-15.2
0	4	5	8.2	7.0
0	4	6	12.1	10.8
0	4	8	7.9	8.1
0	4	9	14.8	16.4
0	5	3	27.6	29.2
0	5	4	20.3	-21.6
0	5	5	29.8	29.2
0	5	6	10.8	-10.5
0	5	7	13.3	-12.8
0	6	3	8.4	-9.2
0	6	4	8.7	8.5
0	6	5	14.2	14.8
0	6	7	11.6	12.4
0	7	4	13.6	-14.0
0	7	5	19.0	18.6
0	7	6	13.5	13.9
0	7	7	10.6	-11.7
0	8	6	8.6	-9.0
0	9	2	9.0	9.1
0	9	3	5.0	-6.1
0	9	4	12.1	-12.0
0	9	6	10.1	10.1
0	9	7	4.9	-4.8
1	1	2	36.2	36.6
1	1	3	41.7	41.2
1	1	4	23.6	23.2
1	1	5	16.5	15.5
1	1	6	32.2	29.7
1	1	9	14.2	-15.4
1	2	1	47.0	48.6
1	2	2	17.4	-18.0
1	2	3	32.4	-31.6
1	2	4	18.4	-18.1
1	2	5	8.1	7.2
1	2	6	8.3	4.3
1	2	8	17.4	16.3
1	2	10	11.0	-12.1
1	3	1	10.3	-10.4
1	3	2	32.2	-33.1
1	3	3	32.7	31.0
1	3	4	52.2	-51.7
1	3	5	31.5	-31.4
1	3	6	7.1	-7.4
1	3	7	9.4	-9.3
1	3	9	6.4	-5.2
1	3	11	8.0	9.8
1	4	2	6.8	-6.5
1	4	3	34.1	34.2
1	4	4	31.3	30.4
1	4	5	9.4	-9.2
1	4	6	7.4	-6.8
1	4	8	6.6	5.3
1	4	9	7.8	-6.4
1	4	10	5.9	-4.9
1	5	1	13.2	-13.6
1	5	2	16.4	-15.8
1	5	3	15.8	15.5
1	5	5	7.0	-7.3
1	5	6	7.1	6.9
1	5	7	10.9	9.7
1	5	8	13.4	13.2
1	6	1	14.8	-14.9
1	6	2	6.1	-5.6
1	6	3	5.6	-5.6
1	6	4	9.4	-8.5
1	6	5	15.7	-15.5
1	7	1	6.0	-5.6
1	7	4	10.4	-10.4
1	7	5	25.6	-24.3
1	7	7	5.2	-6.1
1	8	2	12.9	-12.0
1	8	3	12.5	12.3
1	8	4	12.6	12.8
1	8	6	6.0	5.2
1	8	7	14.0	-13.1
1	9	2	7.3	-6.8
1	9	3	7.7	-8.7
1	9	4	23.6	23.2
1	9	5	23.9	23.0
1	9	6	5.1	-5.1
1	10	1	10.0	10.1
1	10	3	7.5	-7.6
1	10	6	4.2	-3.1
1	11	1	12.5	12.9
2	0	0	63.6	-65.0
2	0	1	20.7	22.1
2	0	2	61.9	61.4
2	0	3	12.6	11.9
2	0	4	14.1	12.5
2	0	8	10.9	9.1
2	0	9	22.9	22.9
2	1	0	53.1	52.7
2	1	1	36.4	36.0
2	1	3	7.6	8.3
2	1	5	13.2	-12.0
2	1	6	22.4	21.4
2	1	8	15.2	-15.0
2	1	10	10.8	-8.4
2	2	0	48.3	48.2
2	2	1	10.1	10.9
2	2	2	62.2	-61.7
2	2	4	10.0	8.6
2	2	6	12.0	11.2
2	2	8	8.1	-7.3
2	2	9	7.7	-8.6
2	3	0	8.7	8.4
2	3	1	6.3	6.9
2	3	2	49.5	50.0
2	3	3	25.4	24.7
2	3	4	29.0	28.9
2	3	5	9.4	9.7
2	3	6	8.0	7.6
2	3	7	5.9	4.6
2	3	8	8.4	-6.0
2	3	9	7.8	8.1
2	4	0	25.6	25.5
2	4	1	17.3	-17.1
2	4	2	31.5	-30.8
2	4	3	33.3	34.3
2	4	4	11.5	10.1
2	4	5	15.6	-13.8
2	5	1	26.8	-25.5
2	5	2	23.5	23.0
2	5	3	18.6	-18.2
2	5	4	26.8	-25.2
2	5	5	17.9	18.6
2	5	6	9.5	8.3
2	5	8	14.6	-14.4
2	6	0	21.7	-21.2
2	6	4	6.3	5.5
2	6	5	21.6	-21.6
2	7	0	11.8	12.0
2	7	1	19.7	-18.2
2	7	3	5.0	-5.5
2	7	4	16.3	-16.2
2	7	5	12.1	-12.0
2	7	6	8.7	-9.2
2	8	2	5.5	5.5
2	8	5	6.1	5.9
2	8	8	5.2	-4.6
2	9	1	8.7	-9.0
2	9	3	13.4	-13.8
2	9	4	9.5	9.4
2	9	5	4.4	4.4
2	9	7	6.1	4.9
2	10	0	4.0	3.4
2	10	4	5.3	-6.1
2	10	6	6.4	5.0
3	1	0	79.5	80.8
3	1	1	114.7	-118.3
3	1	2	43.2	42.2
3	1	4	17.9	17.2
3	1	5	20.1	-18.3
3	1	6	17.1	15.3
3	1	7	15.7	14.9
3	1	8	20.3	-19.8
3	2	1	16.8	17.1
3	2	2	24.8	-23.5
3	2	3	18.1	-16.7
3	2	4	6.1	3.0
3	2	6	18.5	18.4
3	2	7	9.0	9.8
3	2	8	11.8	11.9
3	3	1	21.1	-21.0
3	3	2	11.9	10.3
3	3	3	9.2	11.5
3	3	4	35.9	-33.6
3	3	9	6.6	5.3
3	4	0	21.4	22.1
3	4	1	7.2	6.5
3	4	2	22.2	20.4
3	4	4	19.9	-19.9
3	4	5	15.5	15.7
3	4	6	7.3	6.2
3	4	8	14.0	13.8
3	5	0	14.8	14.2
3	5	2	27.6	27.8
3	5	3	19.1	19.1
3	5	4	6.1	-7.2
3	5	5	5.3	6.4
3	5	6	5.9	-4.7
3	6	0	11.8	12.7
3	6	1	31.2	-29.8
3	6	3	12.8	-11.2
3	6	4	6.6	5.2
3	6	5	19.9	19.3
3	6	6	23.4	-21.7
3	7	0	11.6	-13.1
3	7	1	8.6	-8.2
3	7	2	16.7	17.2
3	7	3	23.7	-23.6
3	7	5	8.3	-9.4
3	8	0	5.3	-4.9
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3	8	3	24.0	22.8
3	8	4	12.8	-12.6
3	8	5	15.3	-13.9
3	8	7	7.6	-6.6
3	9	3	4.5	5.4
3	9	6	7.6	6.4
3	10	0	10.8	-11.1
3	10	5	4.9	5.6
3	11	0	9.8	-9.9
3	11	2	6.8	-5.5
4	0	0	52.8	-53.9
4	0	1	20.6	-19.1
4	0	2	21.9	22.7
4	0	5	15.5	13.8
4	0	6	21.9	-21.1
4	0	7	22.7	-20.7
4	0	8	10.7	11.5
4	1	1	26.5	26.0
4	1	2	32.1	-32.6
4	1	4	8.5	-7.7
4	1	5	7.8	5.2
4	1	6	16.5	-15.5
4	1	7	19.6	-18.8
4	1	8	8.2	-7.4
4	2	1	6.2	6.0
4	2	2	9.6	8.4
4	2	3	36.7	35.6
4	2	4	26.3	-25.7
4	2	6	13.6	12.7
4	3	0	10.8	-10.2
4	3	1	7.3	6.7
4	3	2	20.6	-20.8
4	3	3	8.3	7.5
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4	3	5	15.9	14.5
4	3	6	16.4	15.5
4	3	7	8.7	8.8
4	3	8	11.3	10.0
4	3	9	8.6	-8.2
4	4	0	30.6	-30.1
4	4	1	27.4	-27.4
4	4	2	13.7	12.2
4	4	4	20.4	-20.6
4	4	5	7.3	7.5
4	4	6	11.2	-10.6
4	4	7	10.5	10.7
4	4	8	11.2	11.1
4	5	4	15.6	15.5
4	5	5	12.9	-12.4
4	5	6	7.6	-6.8
4	6	0	18.1	-18.5
4	6	1	25.9	-24.9
4	6	2	5.1	-6.0
4	6	3	11.8	11.6
4	6	6	17.0	15.0
4	7	0	9.4	-9.5
4	7	2	14.3	-14.1
4	7	4	11.0	11.2
4	7	5	5.9	5.9
4	7	6	7.7	-7.5
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4	8	1	11.8	11.0
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5	1	2	20.2	-19.5
5	1	3	14.1	13.3
5	1	5	23.0	21.7
5	1	6	15.3	14.6
5	1	7	11.2	-12.2
5	2	0	88.7	89.7
5	2	1	11.5	-11.1
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5	2	4	12.9	-13.0
5	2	5	6.4	-4.5
5	3	0	20.4	20.5
5	3	1	36.8	37.0
5	3	2	16.4	16.4
5	3	3	11.6	-11.9
5	3	4	11.8	-11.3
5	4	0	43.7	-43.8
5	4	2	40.8	39.4
5	4	4	6.6	5.9
5	4	6	7.0	6.3
5	4	7	6.0	6.6
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5	5	2	8.2	-9.7
5	5	3	11.7	-11.5
5	5	4	19.7	-19.7
5	5	5	12.9	-12.4
5	6	0	9.4	-10.4
5	6	2	6.4	8.2
5	6	3	19.6	-19.8
5	6	4	7.7	-9.4
5	6	5	8.2	-10.1
5	6	6	5.8	6.3
5	7	0	9.4	9.6
5	7	1	21.1	20.2
5	7	2	5.7	5.2
5	7	4	7.1	-5.8
5	8	0	17.3	-18.0
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5	8	2	21.6	21.5
5	8	4	12.8	12.0
5	8	5	10.5	9.3
5	8	6	4.7	-4.8
5	9	0	13.7	-14.9
5	9	1	12.5	-12.4
5	9	3	7.0	8.4
5	9	4	6.3	6.4
5	10	0	9.1	11.0
5	10	2	4.3	-3.4
5	11	0	8.1	8.1
5	11	2	4.7	4.3
6	0	0	9.8	-9.6
6	0	2	10.4	10.4
6	0	3	16.5	17.2
6	0	4	7.3	7.6
6	0	5	34.1	-31.7
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6	1	5	22.3	21.3
6	2	0	28.3	-28.5
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6	2	4	6.9	5.2
6	2	5	13.1	12.7
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6	4	0	13.2	-12.8
6	4	1	23.4	-23.1
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6	4	3	10.3	-10.2
6	4	4	7.6	-6.9
6	4	6	7.0	-5.0
6	5	2	8.2	-8.2
6	5	3	21.1	-22.2
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6	8	1	9.2	8.2
6	8	4	6.3	7.0
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6	9	0	5.4	-4.2
6	9	1	8.0	-8.3
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5	3	-10	10.7	10.4
5	4	-1	10.7	-10.9
5	4	-2	8.1	8.4
5	4	-3	34.7	34.2
5	4	-4	11.2	-11.4
5	4	-5	6.1	6.8
5	4	-8	15.3	15.7
5	4	-12	7.3	5.1
5	5	-1	13.0	-11.2
5	5	-2	26.1	25.3
5	5	-3	8.7	8.3
5	5	-5	35.3	35.1
5	5	-6	17.0	16.6
5	5	-8	11.2	-11.6
5	5	-11	7.3	-7.8
5	5	-12	6.8	-6.9
5	6	-2	12.5	-12.2
5	6	-3	30.2	29.8
5	6	-4	25.7	-26.3
5	6	-7	23.2	-22.6
5	6	-8	10.4	9.5
5	6	-9	8.2	-8.1
5	6	-10	6.6	7.7
5	7	-2	5.0	5.5
5	7	-3	7.9	-8.3
5	7	-4	16.6	-16.2
5	7	-6	22.4	22.4
5	7	-7	9.5	-9.9
5	7	-9	16.8	18.8
5	8	-2	4.8	-5.1
5	8	-3	5.5	5.3
5	8	-5	6.8	-7.3
5	8	-7	24.6	24.4
5	8	-8	18.2	17.3
5	8	-9	4.7	-5.1
5	9	-1	6.8	6.9
5	9	-2	8.3	7.7
5	9	-3	6.3	-6.4
5	9	-5	7.0	-8.2
5	9	-6	13.4	-13.3
5	9	-8	4.5	-2.2
5	9	-9	8.4	-7.7
5	10	-4	4.1	-4.0
5	10	-5	7.4	7.5
5	10	-6	6.4	-6.4
5	10	-7	7.3	-6.0
5	11	-2	4.5	-5.1
5	11	-4	11.1	-10.3
5	11	-5	4.0	3.7
5	12	-2	4.8	-3.6
6	0	-1	31.9	-32.2
6	0	-2	63.5	-63.1
6	0	-3	29.5	28.1
6	0	-5	36.8	-36.8
6	0	-6	31.2	-31.7
6	0	-7	25.1	24.0
6	0	-8	18.7	-18.6
6	0	-9	24.6	-23.1
6	0	-11	13.0	12.9
6	0	-12	9.3	7.9
6	1	-2	60.4	-61.6
6	1	-3	76.6	-76.3
6	1	-4	81.8	-82.2
6	1	-5	36.7	35.5
6	1	-7	22.2	-21.6
6	1	-9	14.5	-14.9
6	1	-10	8.7	-7.8
6	1	-11	13.3	14.1
6	1	-12	22.2	26.9
6	2	-1	67.1	68.2
6	2	-2	14.4	-14.8
6	2	-3	27.9	28.5
6	2	-5	33.6	-32.2
6	2	-7	35.8	34.0
6	2	-8	26.6	26.8
6	2	-10	24.9	26.2
6	2	-11	11.9	-11.1
6	2	-13	8.0	9.4
6	3	-1	8.9	-8.6
6	3	-2	26.7	-27.8
6	3	-3	25.3	-25.0
6	3	-5	11.6	11.3
6	3	-6	40.8	-40.8
6	3	-7	33.5	33.6
6	3	-8	33.2	32.6
6	3	-9	9.4	-9.4
6	3	-12	7.3	9.8
6	4	-1	22.6	23.1
6	4	-3	9.1	9.1
6	4	-4	13.6	-12.9
6	4	-5	20.6	21.7
6	4	-6	29.4	28.5
6	4	-7	26.0	-25.4
6	4	-8	8.7	-8.8
6	4	-9	45.0	-44.0
6	4	-10	10.3	10.4
6	4	-12	6.0	-5.5
6	5	-1	8.7	-8.9
6	5	-2	16.2	15.8
6	5	-3	14.6	-14.6
6	5	-5	18.6	18.4
6	5	-7	12.6	-11.5
6	5	-11	14.6	15.1
6	5	-12	10.0	-11.1
6	6	-2	8.3	-6.9
6	6	-3	20.6	20.5
6	6	-4	12.0	10.7
6	6	-5	12.7	12.6
6	6	-8	10.2	-10.5
6	6	-9	8.0	-9.0
6	6	-10	5.0	5.6
6	7	-1	13.3	13.4
6	7	-4	10.7	10.5
6	7	-5	5.3	6.0
6	7	-6	6.5	6.9
6	7	-8	5.0	-4.1
6	8	-1	14.8	-14.6
6	8	-2	8.9	9.2
6	8	-3	6.5	6.4
6	8	-5	7.6	-7.3
6	8	-7	17.2	15.6
6	8	-9	5.3	5.4
6	9	-1	6.5	6.6
6	9	-2	16.4	16.6
6	9	-3	8.3	8.0
6	9	-5	8.3	7.9
6	9	-6	9.6	-10.1
6	9	-9	7.9	-7.3
6	10	-1	5.2	-5.5
6	10	-2	4.2	4.5
6	10	-3	4.2	-3.8
6	10	-4	16.1	-16.8
6	10	-5	10.0	-9.4
6	10	-6	8.6	8.7
6	10	-7	6.7	-6.4
6	10	-9	4.5	4.1
6	11	-3	10.4	-10.1
6	11	-4	5.0	-5.5
6	12	-1	4.3	-3.4
7	1	-1	7.8	-8.9
7	1	-2	30.2	28.1
7	1	-3	46.3	-45.2
7	1	-5	44.4	43.3
7	1	-6	21.9	-20.7
7	1	-7	12.5	10.6
7	1	-9	16.3	-15.6
7	1	-12	8.9	-9.9
7	1	-13	12.5	-11.9
7	1	-14	13.1	16.2
7	2	-1	66.2	-66.8
7	2	-2	21.5	20.7
7	2	-3	15.4	-15.2
7	2	-4	19.5	20.5
7	2	-6	8.5	7.4
7	2	-7	11.0	-11.7
7	2	-8	14.4	14.9
7	2	-9	7.2	6.5
7	2	-10	18.0	16.9
7	2	-12	6.9	8.2
7	2	-13	7.1	7.5
7	3	-1	9.0	-8.2
7	3	-2	22.9	24.0
7	3	-3	21.1	21.1
7	3	-4	14.4	13.5
7	3	-5	16.9	-17.2
7	3	-6	10.5	9.2
7	3	-7	12.0	11.7
7	3	-8	6.6	-6.2
7	3	-9	7.2	6.1
7	3	-10	6.5	7.4
7	3	-11	9.4	9.3
7	3	-12	9.0	-9.1
7	3	-13	6.9	6.0
7	4	-1	9.1	7.8
7	4	-2	5.4	6.3
7	4	-3	28.3	-29.9
7	4	-4	17.6	-17.3
7	4	-6	5.5	-5.9
7	4	-7	8.7	7.9
7	4	-9	20.3	19.9
7	4	-10	18.0	-18.0
7	4	-12	6.8	7.8
7	5	-1	9.7	-10.6
7	5	-2	18.0	-18.4
7	5	-3	25.7	-26.2
7	5	-4	7.7	-8.1
7	5	-5	14.8	-14.5
7	5	-6	13.6	-14.6
7	5	-9	7.3	-8.5
7	5	-11	6.3	7.6
7	6	-2	21.1	20.8
7	6	-4	15.5	16.6
7	6	-5	14.3	12.7
7	6	-6	7.0	-6.7
7	6	-7	5.0	-3.5
7	6	-8	13.0	-11.9
7	6	-9	14.9	14.7
7	6	-10	14.8	-15.2
7	7	-3	11.4	13.4
7	7	-4	13.6	13.9
7	7	-5	8.6	9.1
7	7	-6	6.3	-7.8
7	7	-7	8.0	-8.2
7	7	-9	10.5	9.7
7	7	-10	13.1	13.9

Table 1 (*cont.*)

7	8	-1	25.1	-24.9
7	8	-2	15.5	14.6
7	8	-7	24.6	-22.9
7	8	-9	14.9	14.8
7	8	-10	14.9	-14.1
7	8	-11	6.1	-6.1
7	9	-2	4.7	3.7
7	9	-3	4.3	-3.4
7	9	-4	9.2	-9.6
7	9	-5	9.8	-9.9
7	9	-6	12.3	11.9
7	9	-7	14.0	13.4
7	9	-9	8.3	-7.4
7	9	-10	11.8	-10.3
7	10	-1	6.5	-6.0
7	10	-2	7.1	7.8
7	10	-5	4.1	-4.5
7	10	-7	8.2	8.4
7	11	-3	8.8	8.5
8	0	-1	19.7	-20.5
8	0	-2	66.5	67.0
8	0	-3	17.7	-17.5
8	0	-5	99.6	-99.2
8	0	-6	83.4	-83.1
8	0	-7	57.2	55.2
8	0	-8	8.3	-7.1
8	0	-10	9.8	8.1
8	0	-11	9.5	-9.2
8	0	-12	9.0	-9.2
8	0	-15	7.1	-10.1
8	1	-1	51.1	-51.9
8	1	-2	9.0	-8.0
8	1	-3	37.5	37.5
8	1	-4	28.5	-28.8
8	1	-5	26.7	25.4
8	1	-6	68.3	65.9
8	1	-7	12.7	12.1
8	1	-8	21.9	20.0
8	1	-9	8.0	6.2
8	1	-10	13.3	12.3
8	1	-12	18.7	-21.0
8	1	-13	10.6	-12.4
8	2	-1	16.0	-14.2
8	2	-2	12.7	-11.2
8	2	-4	20.0	20.4
8	2	-6	20.5	20.2
8	2	-7	10.5	11.2
8	2	-8	19.0	-19.0
8	2	-10	28.5	-28.0
8	2	-11	15.3	15.0
8	2	-12	12.7	13.0
8	3	-3	6.4	6.7
8	3	-4	6.7	-6.3
8	3	-6	30.1	29.6
8	3	-7	23.2	23.3
8	3	-8	8.0	-6.8
8	3	-9	12.9	-12.5
8	3	-10	15.3	15.2
8	4	-1	23.5	-24.2
8	4	-3	17.0	17.0
8	4	-5	17.2	-17.4
8	4	-6	20.9	-21.1
8	4	-7	12.0	11.9
8	4	-8	21.7	20.6
8	4	-10	7.1	-5.8
8	4	-11	10.5	11.3
8	4	-13	11.2	-10.1
8	5	-1	14.2	13.7
8	5	-2	14.9	-14.2
8	5	-4	26.1	-24.7
8	5	-5	11.7	-12.0
8	5	-6	41.5	40.5
8	5	-10	7.8	-8.1
8	6	-1	12.1	-12.1
8	6	-2	5.0	5.0
8	6	-4	10.2	9.9
8	6	-5	14.1	13.8
8	6	-6	17.0	16.6
8	6	-7	5.2	5.3
8	6	-8	10.6	-10.0
8	6	-11	5.0	-3.6
8	7	-1	8.3	7.5
8	7	-2	7.0	6.7
8	7	-3	12.6	12.3
8	7	-4	11.5	12.5
8	7	-5	10.5	-10.8
8	7	-6	20.6	-21.5
8	7	-7	18.9	-17.6
8	7	-8	5.7	5.8
8	7	-9	9.2	-8.3
8	7	-11	4.8	4.8
8	8	-2	12.0	11.9
8	8	-4	8.3	-8.6
8	8	-8	7.6	-6.7
8	9	-1	6.5	7.6
8	9	-2	5.9	-6.8
8	9	-4	6.0	-6.4
8	9	-7	6.2	-4.8
8	9	-8	5.3	-4.0
8	9	-9	5.1	-4.9
8	9	-10	5.1	4.9
8	9	-11	5.3	2.9
8	10	-2	6.4	-6.9
8	10	-5	5.1	-5.3
8	10	-6	7.3	-6.8
8	11	-1	4.0	2.4
8	11	-3	3.9	3.2
8	11	-4	4.2	-4.1
8	11	-5	5.0	4.8
8	11	-6	6.9	7.0
9	1	-1	18.6	17.4
9	1	-2	31.0	-30.4
9	1	-3	12.1	13.1
9	1	-4	6.8	-7.1
9	1	-6	27.4	-25.7
9	1	-7	19.6	-20.5
9	1	-8	21.2	18.7
9	1	-9	22.8	-22.0
9	1	-11	7.3	-6.2
9	1	-13	8.3	8.6
9	1	-15	6.3	7.1
9	2	-1	64.0	64.1
9	2	-2	30.8	31.3
9	2	-3	12.1	-12.0
9	2	-4	12.1	-10.9
9	2	-5	15.7	16.1
9	2	-7	24.9	-24.9
9	2	-8	38.8	37.8
9	2	-9	28.4	-28.0
9	2	-11	8.1	6.8
9	2	-12	16.4	16.1
9	3	-1	33.8	34.0
9	3	-2	11.4	-12.4
9	3	-3	31.8	-32.2
9	3	-4	15.8	16.1
9	3	-5	9.5	10.0
9	3	-6	23.1	22.8
9	3	-7	7.2	-6.9
9	3	-8	15.5	17.0
9	3	-9	7.2	-6.5
9	3	-10	17.5	16.7
9	3	-11	20.9	19.9
9	3	-12	19.8	-19.4
9	3	-14	7.8	-8.6
9	4	-1	25.2	-24.0
9	4	-2	16.8	-18.2
9	4	-4	12.9	14.2
9	4	-5	32.4	32.7
9	4	-6	6.9	-5.7
9	4	-7	19.3	-20.6
9	4	-10	7.8	-8.3
9	4	-11	8.5	-7.6
9	4	-12	8.2	-7.4
9	5	-2	9.7	-9.7
9	5	-3	17.5	16.9
9	5	-4	19.5	20.6
9	5	-5	5.7	-3.8
9	5	-6	13.0	13.6
9	5	-7	10.5	-10.6
9	5	-9	17.6	-17.3
9	5	-11	8.3	8.4
9	5	-12	10.5	-11.3
9	6	-5	6.6	-8.2
9	6	-6	13.5	-14.5
9	6	-9	16.4	15.4
9	6	-11	11.7	11.6
9	6	-12	8.5	8.5
9	7	-1	13.1	13.5
9	7	-5	11.1	-12.1
9	7	-6	7.2	-7.0
9	7	-7	33.7	34.2
9	7	-8	8.7	9.1
9	7	-9	9.8	-9.5
9	7	-10	9.8	9.9
9	7	-13	5.9	-4.7
9	8	-1	11.4	-12.5
9	8	-2	11.7	-12.2
9	8	-4	5.1	5.0
9	8	-5	5.9	5.2
9	8	-6	6.2	-7.7
9	8	-8	10.9	11.6
9	8	-11	11.4	-10.9
9	8	-12	8.3	-9.4
9	9	-1	19.4	-20.2
9	9	-3	13.8	14.9
9	9	-4	4.3	-4.4
9	9	-6	9.5	-8.8
9	9	-7	12.5	-12.8
9	9	-10	8.8	-8.8
9	10	-1	6.3	7.2
9	10	-4	7.2	-7.0
9	10	-6	8.0	7.8
9	10	-7	8.9	-8.8
9	11	-5	6.5	-6.7
10	0	-1	34.4	-34.0
10	0	-2	28.8	-29.8
10	0	-3	19.3	-18.7
10	0	-4	19.1	-18.6
10	0	-5	35.9	-30.0
10	0	-6	47.7	-46.9
10	0	-8	88.3	89.4
10	0	-12	27.5	26.6
10	0	-14	6.1	8.4
10	1	-1	22.8	24.0
10	1	-2	24.5	24.5
10	1	-4	10.8	11.8
10	1	-5	35.8	-35.3
10	1	-6	45.4	45.0
10	1	-7	59.2	58.4
10	1	-8	11.1	10.9
10	1	-11	12.7	-12.5
10	1	-12	8.5	11.0
10	1	-13	27.3	29.5
10	1	-14	8.3	-10.5
10	2	-1	15.5	-15.0
10	2	-2	28.1	28.0
10	2	-3	7.2	7.1
10	2	-5	11.7	11.0
10	2	-6	35.0	-34.6
10	2	-7	5.9	5.4
10	2	-8	14.5	12.9
10	2	-11	7.9	7.3
10	2	-12	6.9	-7.9
10	2	-13	6.6	-7.5
10	3	-1	13.2	-13.9
10	3	-3	19.5	-19.6
10	3	-4	25.0	-25.5
10	3	-6	9.2	8.8
10	3	-7	23.6	-24.3
10	3	-9	15.4	14.9
10	3	-10	13.8	-13.9
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10	4	-2	7.9	6.8
10	4	-4	8.9	9.1
10	4	-5	12.9	13.5
10	4	-7	14.0	14.0
10	4	-8	14.8	-15.1
10	4	-10	32.0	-31.3
10	5	-1	9.2	-8.2
10	5	-2	8.6	9.8
10	5	-3	10.3	10.4
10	5	-5	15.4	16.5
10	5	-6	7.3	-6.3
10	5	-7	18.8	17.6
10	5	-8	16.8	-16.6
10	5	-9	7.4	8.8
10	5	-10	5.5	4.8
10	5	-12	14.1	13.5
10	5	-13	13.9	-12.6
10	6	-4	8.1	9.4
10	6	-5	9.0	10.0
10	6	-7	12.9	-13.7
10	6	-10	6.6	-6.2
10	6	-11	5.8	-6.8
10	6	-12	6.5	6.8
10	6	-14	5.4	-5.2
10	7	-1	10.1	-10.0
10	7	-2	19.2	19.7
10	7	-4	15.9	-15.4
10	7	-5	7.2	7.3
10	7	-6	7.3	7.6
10	7	-7	8.2	8.2
10	7	-8	7.8	-8.0
10	7	-9	8.8	8.7
10	7	-10	6.7	-6.3
10	7	-12	7.7	9.3
10	7	-13	6.9	-6.1
10	8	-2	10.3	-8.9
10	8	-3	4.5	3.6
10	8	-4	7.1	7.3
10	8	-5	6.1	5.5
10	8	-6	5.8	-6.1
10	8	-8	9.7	10.8
10	8	-9	6.1	-5.8
10	9	-1	9.4	-9.3
10	9	-2	7.4	7.7
10	9	-3	6.4	7.5
10	9	-5	5.2	-5.8
10	9	-7	12.3	-12.7
10	9	-8	6.6	-6.9
10	9	-10	5.3	-5.0
10	10	-2	4.3	-4.3
10	10	-3	6.6	-6.2
10	10	-5	11.6	-12.0
10	10	-6	7.9	-7.6
10	10	-7	9.2	9.1
10	10	-9	4.2	3.9
10	11	-6	4.1	-1.6
10	11	-7	8.6	8.1
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11	1	-3	12.1	10.4
11	1	-5	11.4	11.8
11	1	-6	10.7	10.3
11	1	-7	11.5	12.4
11	1	-9	7.7	7.3
11	2	-1	7.8	-7.2
11	2	-2	12.2	-11.5
11	2	-3	30.6	31.0
11	2	-4	5.9	6.9
11	2	-5	16.2	-16.3
11	2	-6	22.0	22.1
11	2	-9	12.0	11.8
11	2	-11	16.5	16.4
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11	3	-1	20.5	21.4
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11	3	-5	5.9	6.3
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11	5	-11	8.7	-9.0
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11	6	-3	11.9	11.9
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11	6	-5	5.6	6.8
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11	6	-7	12.3	-12.6
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11	7	-3	8.3	-8.6
11	7	-4	9.9	-11.4
11	7	-5	5.7	5.4
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11	7	-7	18.7	-19.5
11	7	-8	8.2	-8.5
11	7	-10	6.3	5.9
11	7	-11	14.0	11.5
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11	8	-2	19.9	-19.7
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11	8	-4	7.4	7.9
11	8	-5	5.9	-5.3
11	8	-6	5.3	3.0
11	8	-8	9.1	-9.4
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11	8	-12	13.3	-12.2
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11	9	-4	7.2	6.4
11	9	-5	5.7	-5.5
11	9	-7	12.1	12.1
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11	9	-11	10.6	-9.6
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11	10	-9	4.9	3.5
12	0	-1	13.2	13.5
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12	0	-12	13.7	-13.2
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12	1	-5	14.4	14.5
12	1	-6	23.9	23.4
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12	2	-10	10.6	-9.3
12	2	-11	8.4	-8.0
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12	2	-13	14.6	14.1
12	2	-14	6.7	-2.1
12	3	-2	8.9	10.5
12	3	-3	6.0	5.6
12	3	-4	6.2	7.2
12	3	-5	6.0	5.2
12	3	-6	6.1	7.7
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12	3	-10	11.9	-12.1
12	4	-2	8.1	-7.6
12	4	-4	16.0	17.0
12	4	-6	8.0	-9.9
12	4	-7	19.1	-19.8
12	4	-8	5.8	6.7
12	4	-9	21.4	22.0
12	4	-10	6.3	-6.6
12	4	-14	6.5	-5.7
12	5	-4	6.4	-8.0
12	5	-7	16.2	16.8
12	5	-8	17.4	17.7
12	5	-10	7.0	-7.8
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12	6	-4	10.1	10.1
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12	6	-9	22.7	-22.1
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12	7	-5	6.3	5.2
12	7	-6	5.2	-6.3
12	7	-7	23.7	-24.1
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12	9	-5	5.7	-5.6
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13	1	-2	9.1	9.6
13	1	-7	19.0	-18.4
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13	1	-13	9.1	7.9
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13	8	-3	6.4	-7.1
13	8	-4	12.1	-12.2
13	8	-5	11.5	12.3
13	8	-6	6.8	6.3
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13	9	-8	5.3	-4.1
14	0	-1	10.5	-10.5
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14	0	-6	11.1	9.5
14	0	-7	13.2	13.3
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14	0	-14	11.7	-12.4
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14	1	-8	14.1	14.2
14	1	-9	6.8	7.3
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14	1	-11	21.4	-20.7
14	1	-12	13.9	-13.4
14	1	-13	7.0	5.3
14	1	-14	14.9	13.4
14	2	-4	14.7	-14.0
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14	3	-1	9.1	8.5
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14	4	-1	7.2	9.2
14	4	-2	6.8	6.2
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14	4	-9	11.2	-13.0
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14	5	-6	7.2	7.4
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15	3	-11	6.6	-6.0
15	3	-13	20.7	19.8
15	3	-15	14.6	-13.9
15	4	-2	8.5	8.8
15	4	-6	6.1	6.5
15	4	-8	6.6	5.7
15	4	-9	6.0	5.2
15	4	-12	5.4	-4.1
15	5	-7	11.1	-12.6
15	5	-8	5.5	-5.1
15	5	-12	7.7	-8.3
15	5	-14	7.7	6.7
15	6	-6	6.5	6.8
15	6	-8	7.8	-8.6
15	7	-5	10.7	-12.4
15	7	-7	11.8	11.7
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15	7	-11	5.0	3.5
15	8	-6	8.8	9.7
16	0	-9	18.9	21.1
16	0	-10	23.4	24.6
16	0	-11	23.5	23.5
16	0	-12	7.6	-9.0
16	0	-13	19.6	-19.9
16	0	-14	8.5	-7.3
16	1	-2	8.9	-10.5
16	1	-4	9.2	-9.3
16	1	-6	10.8	10.9
16	1	-7	23.1	23.1
16	1	-11	26.6	-26.9
16	1	-12	9.2	-9.1
16	1	-14	15.5	-14.0
16	2	-3	11.9	12.0
16	2	-4	8.5	-9.0
16	2	-6	12.9	13.4
16	2	-8	6.6	-4.1
16	2	-10	9.5	-8.6
16	2	-11	11.1	-11.1
16	2	-15	8.3	5.8
16	3	-3	17.0	17.4
16	3	-7	6.1	4.9
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16	4	-8	7.7	-7.2
16	4	-10	15.9	15.1
16	5	-5	6.4	-7.7
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16	5	-10	9.4	7.5
16	5	-11	17.5	-16.1
16	5	-12	10.0	-10.1
16	6	-4	6.6	-6.6
16	6	-7	7.6	-8.8
16	6	-9	5.7	5.0
16	6	-10	13.1	-12.4
16	6	-11	5.9	-4.9
16	6	-12	5.9	6.4
16	7	-8	7.3	-8.2
16	7	-10	7.2	6.6
17	1	-3	16.2	14.8
17	1	-5	6.6	4.1
17	1	-8	10.7	-11.2
17	1	-10	6.3	6.6
17	1	-11	19.1	-17.3
17	1	-13	15.2	14.4
17	2	-3	18.6	19.0
17	2	-4	5.9	-3.6
17	2	-6	9.7	-11.0
17	2	-9	9.7	-9.9
17	2	-13	15.0	-13.7
17	2	-14	6.5	5.3
17	3	-5	9.4	-10.6
17	3	-9	8.8	-8.9
17	3	-12	6.7	6.8
17	3	-14	8.4	-7.8
17	4	-4	8.8	8.8
17	4	-7	15.8	17.1
17	4	-13	6.2	3.7
17	5	-5	6.1	-5.9
17	5	-7	9.4	9.4
17	5	-9	10.8	-11.3
17	6	-6	6.0	-7.2
17	6	-7	8.4	-8.2
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17	6	-11	9.4	9.0
17	6	-12	6.0	-4.5
18	0	-5	9.0	11.7
18	0	-7	8.3	7.5
18	0	-11	15.4	16.8
18	0	-12	13.6	-14.3
18	0	-13	22.5	-22.1
18	0	-14	8.9	9.2
18	1	-5	6.7	7.9
18	1	-7	19.6	-18.8
18	1	-12	13.9	-14.1
18	1	-13	8.3	-6.1
18	1	-14	12.4	11.9
18	2	-8	11.6	-13.0
18	2	-9	7.6	6.6
18	2	-10	9.3	7.1
18	3	-6	5.7	-4.8
18	3	-8	11.1	10.0
18	3	-9	6.4	2.2
18	3	-11	11.0	-9.7
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18	4	-6	7.5	7.7
18	4	-10	11.0	-10.6
18	4	-12	7.1	-6.7
18	5	-8	12.7	-13.5
18	5	-9	5.1	5.0
19	1	-7	9.2	6.5
19	1	-8	6.2	-4.5
19	1	-12	7.0	7.2
19	2	-7	8.9	-8.7
19	2	-8	6.4	-7.5
19	2	-10	12.8	12.5
19	2	-13	10.3	9.3
19	3	-8	9.4	10.5
19	3	-9	8.9	9.8
19	3	-11	7.2	-6.5
20	0	-10	8.0	8.4

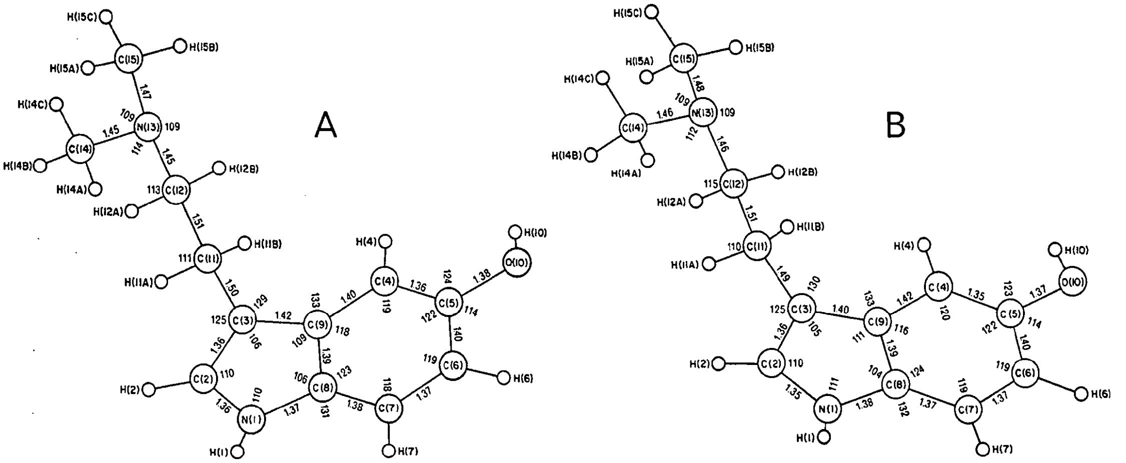

Fig. 1. Atom numbering, bond lengths (Å) and bond angles (°) for non-hydrogen atoms in molecules *A* (left) and *B* (right) of bufotenine [5-hydroxy-(*N*,*N*)-dimethyltryptamine].

sponding e.s.d.'s. The mean e.s.d. of the positional coordinates was 0·006 Å for non-hydrogen atoms and 0·05 Å for the hydrogen coordinates. Isotropic temperature factors of the hydrogen atoms were set equal to those atoms to which they were covalently bound. These B values, ranging from 3·1 to 5·6 Å^2, were not refined.

Table 2. *Final fractional atomic coordinates and their estimated standard deviations (in parentheses)*

Values are $\times 10^4$ for non-hydrogen atoms and $\times 10^3$ for hydrogen.

Molecule *A*

	x/a	y/b	z/c
N(1)	−673 (3)	7915 (4)	82 (3)
C(2)	−379 (3)	9012 (5)	529 (5)
C(3)	465 (3)	8978 (5)	1754 (4)
C(4)	1433 (3)	7185 (4)	3162 (4)
C(5)	1425 (3)	6004 (5)	3150 (4)
C(6)	677 (3)	5365 (5)	2077 (5)
C(7)	−63 (3)	5937 (5)	1001 (4)
C(8)	−52 (3)	7130 (5)	1012 (4)
C(9)	676 (3)	7780 (4)	2067 (4)
O(10)	2126 (2)	5333 (3)	4181 (3)
C(11)	991 (3)	10018 (5)	2579 (4)
C(12)	561 (3)	10361 (5)	3164 (4)
N(13)	1099 (3)	11306 (4)	4051 (3)
C(14)	1008 (4)	12398 (5)	3482 (5)
C(15)	722 (4)	11461 (5)	4701 (5)
H(1)	−122 (3)	774 (4)	−58 (4)
H(2)	−68 (3)	973 (4)	7 (4)
H(4)	200 (3)	759 (4)	387 (4)
H(6)	70 (3)	446 (4)	213 (4)
H(7)	−59 (3)	552 (4)	28 (4)
H(10)	270 (3)	578 (4)	477 (4)
H(11*A*)	93 (3)	1075 (4)	209 (4)
H(11*B*)	170 (3)	985 (4)	319 (4)
H(12*A*)	−18 (3)	1061 (4)	245 (4)
H(12*B*)	61 (3)	966 (4)	363 (4)
H(14*A*)	131 (3)	1229 (4)	314 (4)
H(14*B*)	33 (3)	1261 (4)	286 (4)
H(14*C*)	135 (3)	1310 (4)	407 (4)
H(15*A*)	−1 (3)	1166 (4)	417 (4)
H(15*B*)	85 (3)	1065 (4)	512 (4)
H(15*C*)	108 (3)	1214 (4)	528 (4)

Table 2 (*cont.*)

Molecule *B*

	x/a	y/b	z/c
N(1)	3610 (3)	1361 (4)	4523 (4)
C(2)	3761 (4)	305 (5)	4259 (5)
C(3)	3607 (3)	363 (5)	3186 (4)
C(4)	3105 (3)	2141 (4)	1765 (4)
C(5)	2874 (3)	3280 (4)	1626 (5)
C(6)	2829 (3)	3876 (5)	2445 (5)
C(7)	3077 (3)	3301 (5)	3463 (5)
C(8)	3325 (3)	2151 (5)	3613 (4)
C(9)	3339 (3)	1520 (4)	2790 (4)
O(10)	2636 (2)	3941 (3)	662 (3)
C(11)	3643 (3)	−642 (4)	2559 (4)
C(12)	2740 (3)	−1400 (5)	1958 (4)
N(13)	2604 (3)	−2309 (4)	1141 (4)
C(14)	3450 (4)	−3101 (5)	1797 (5)
C(15)	1701 (4)	−2971 (5)	623 (5)
H(1)	354 (3)	149 (4)	500 (4)
H(2)	394 (3)	−41 (4)	467 (4)
H(4)	318 (3)	167 (4)	124 (4)
H(6)	268 (3)	475 (4)	235 (4)
H(7)	295 (3)	375 (4)	396 (4)
H(10)	272 (3)	351 (4)	31 (4)
H(11*A*)	424 (3)	−115 (4)	314 (4)
H(11*B*)	371 (3)	−31 (4)	202 (4)
H(12*A*)	272 (3)	−181 (4)	254 (4)
H(12*B*)	220 (3)	−89 (4)	150 (4)
H(14*A*)	406 (3)	−266 (4)	207 (4)
H(14*B*)	362 (3)	−351 (4)	252 (4)
H(14*C*)	326 (3)	−385 (4)	130 (4)
H(15*A*)	165 (3)	−335 (4)	122 (4)
H(15*B*)	115 (3)	−233 (4)	11 (4)
H(15*C*)	163 (3)	−369 (4)	16 (4)

The atomic scattering factors were taken from *International Tables for X-ray Crystallography* (1962). The structure amplitudes were given unit weight throughout, because of the counter strategy mentioned. No correction terms for anomalous dispersion were introduced. Observed and calculated structure factors from the last cycle of refinement are listed in Table 1. Positional coordinates and thermal parameters for the final structure are given in Tables 2 and 3.

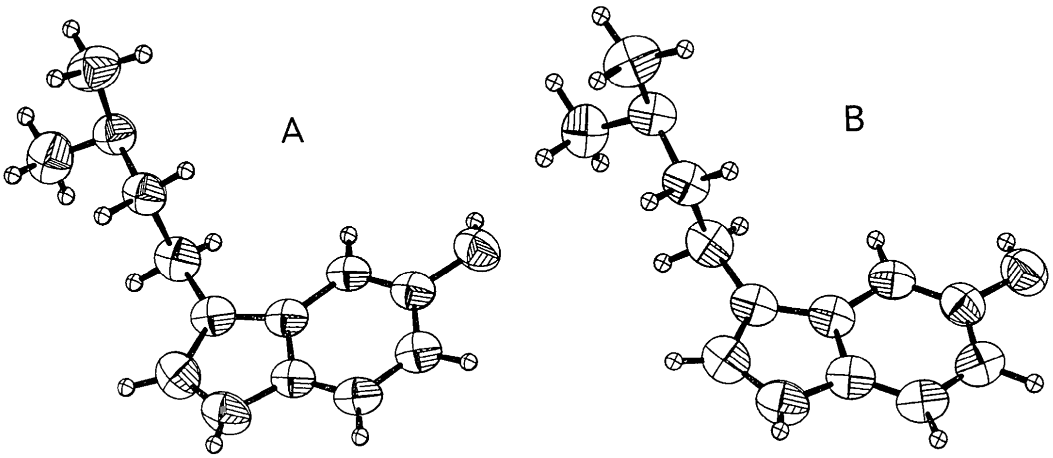

Fig. 2. Molecular conformation of molecules *A* (left) and *B* (right) of bufotenine. The non-hydrogen atoms are represented by 50% probability thermal ellipsoids and the hydrogen atoms indicated by small spheres with a radius of 0·1 Å. The drawings were performed using the program *ORTEP* (Johnson, 1970).

Table 3. *Anisotropic thermal parameters and their standard deviations (in parentheses)*

β_{ij} are the coefficients in the expression:

$$\exp\left[-(\beta_{11}h^2+\beta_{22}k^2+\beta_{33}l^2+\beta_{12}hk+\beta_{13}hl+\beta_{23}kl)\times 10^{-4}\right].$$

Molecule *A*

	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
N(1)	39 (2)	144 (11)	79 (4)	−12 (6)	52 (5)	−8 (8)
C(2)	47 (3)	115 (11)	108 (6)	−6 (7)	83 (7)	6 (10)
C(3)	35 (3)	115 (11)	86 (5)	−16 (6)	73 (6)	−32 (9)
C(4)	35 (3)	109 (11)	72 (5)	−16 (6)	69 (6)	−30 (8)
C(5)	42 (3)	117 (11)	84 (5)	−5 (6)	87 (6)	−10 (8)
C(6)	52 (3)	109 (10)	102 (6)	−22 (7)	102 (7)	−30 (9)
C(7)	41 (3)	128 (11)	81 (5)	−26 (6)	77 (7)	−46 (9)
C(8)	34 (3)	112 (11)	79 (5)	−16 (6)	72 (6)	−22 (9)
C(9)	32 (2)	112 (11)	83 (5)	−3 (6)	79 (6)	−18 (8)
O(10)	57 (2)	124 (10)	84 (4)	3 (4)	74 (5)	10 (6)
C(11)	49 (3)	118 (11)	103 (5)	−13 (6)	96 (7)	−6 (9)
C(12)	48 (3)	111 (10)	92 (5)	0 (6)	83 (7)	2 (9)
N(13)	45 (2)	104 (10)	86 (4)	−7 (5)	72 (5)	−15 (7)
C(14)	66 (3)	164 (12)	128 (6)	−3 (8)	132 (8)	−55 (11)
C(15)	66 (4)	111 (11)	140 (7)	−7 (7)	114 (8)	−16 (10)

Molecule *B*

	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
N(1)	76 (3)	142 (11)	102 (5)	−23 (6)	137 (7)	−25 (8)
C(2)	66 (3)	123 (11)	116 (6)	−4 (7)	128 (8)	11 (10)
C(3)	48 (3)	114 (11)	92 (5)	−7 (6)	96 (6)	−11 (9)
C(4)	38 (3)	106 (11)	88 (5)	−17 (6)	78 (6)	−26 (8)
C(5)	41 (3)	107 (11)	98 (5)	−9 (6)	77 (7)	2 (9)
C(6)	59 (3)	108 (11)	129 (6)	−12 (7)	128 (8)	−39 (10)
C(7)	59 (3)	121 (11)	114 (6)	−35 (7)	128 (8)	−51 (9)
C(8)	53 (3)	115 (11)	108 (5)	−24 (7)	118 (7)	−21 (9)
C(9)	39 (3)	107 (11)	96 (5)	−9 (6)	92 (6)	−10 (9)
O(10)	83 (2)	121 (10)	100 (4)	18 (5)	115 (5)	18 (6)
C(11)	52 (3)	120 (11)	113 (6)	2 (6)	112 (7)	7 (8)
C(12)	55 (3)	117 (10)	103 (5)	12 (6)	108 (7)	−3 (9)
N(13)	55 (3)	114 (10)	103 (4)	−10 (5)	110 (6)	−17 (7)
C(14)	85 (4)	112 (10)	148 (7)	17 (7)	174 (9)	17 (10)
C(15)	86 (4)	136 (11)	167 (7)	−53 (8)	193 (10)	−60 (11)

Table 4. *Equations of the best planes with the formula $m_1X+m_2Y+m_3Z=d$ in orthogonal space*

Plane	m_1	m_2	m_3	d
Molecule *A*				
Pyrrole ring	0·966209	−0·002604	−0·257749	−1·270702
Benzene ring	0·962525	−0·002828	−0·271176	−1·291843
Indole nucleus	0·964117	−0·003775	−0·265458	−1·274719
Molecule *B*				
Pyrrole ring	0·815460	0·237658	0·527771	4·736325
Benzene ring	0·800441	0·246412	0·546419	4·773360
Indole nucleus	0·805692	0·243896	0·539792	4·764162

Deviations (in Å) from the best planes.
Distances marked with asterisks refer to atoms defining the plane.

Planes	Pyrrole ring		Benzene ring		Indole nucleus	
Molecule	*A*	*B*	*A*	*B*	*A*	*B*
N(1)	0·012*	0·009*	0·037	0·043	0·021*	0·028*
C(2)	−0·010*	−0·006*	0·008	0·003	−0·007*	−0·004*
C(3)	0·004*	0·001*	0·003	−0·022	−0·003*	−0·018*
C(4)	0·021	0·039	−0·001*	−0·000*	0·004*	0·011*
C(5)	0·026	0·041	0·004*	0·014*	0·010*	0·022*
C(6)	0·001	−0·026	−0·004*	−0·017*	−0·005*	−0·022*
C(7)	−0·011	−0·026	0·001*	0·005*	−0·007*	−0·008*
C(8)	−0·009*	−0·009*	0·002*	0·009*	−0·008*	0·000*
C(9)	0·003*	0·005*	−0·002*	−0·012*	−0·005*	−0·009*
O(10)	0·023	0·68	−0·014	0·022	−0·001	0·037
C(11)	−0·064	−0·096	−0·077	−0·151	−0·080	−0·136
C(12)	−1·503	−1·504	−1·520	−1·563	−1·521	−1·547
N(13)	−1·623	−1·787	−1·653	−1·879	−1·650	−1·852

Description and discussion of the structure

Bond lengths and bond angles with estimated standard deviations are given in Tables 4, 5 and 6. The atomic numbering system is given in Fig. 1, in which the indole nuclei are labelled in accordance with international rules. The configurations of the two bufotenine molecules are represented in Fig. 2 which shows the thermal ellipsoids of the non-hydrogen atoms. The hydrogen atoms are indicated by small spheres. Hereafter the two molecules of the asymmetric unit are referred to as *A* and *B*. Interatomic distances and angles of the latter are given within parentheses.

Table 5. *Interatomic distances and estimated standard deviations (in parentheses)*

	Molecule *A*	Molecule *B*
N(1)–C(2)	1·356 (7) Å	1·353 (7) Å
C(2)–C(3)	1·361 (7)	1·363 (6)
C(3)–C(9)	1·422 (7)	1·404 (7)
C(9)–C(8)	1·390 (6)	1·393 (6)
C(8)–N(1)	1·366 (6)	1·377 (7)
C(9)–C(4)	1·398 (6)	1·417 (6)
C(4)–C(5)	1·361 (7)	1·351 (7)
C(5)–C(6)	1·404 (7)	1·400 (6)
C(6)–C(7)	1·365 (7)	1·373 (7)
C(7)–C(8)	1·375 (8)	1·369 (8)
C(5)–O(10)	1·378 (6)	1·369 (6)
C(3)—C(11)	1·498 (7)	1·489 (7)
C(11)–C(12)	1·514 (4)	1·514 (5)
C(12)–N(13)	1·450 (6)	1·461 (6)
N(13)–C(14)	1·447 (7)	1·464 (6)
N(13)–C(15)	1·474 (4)	1·475 (5)
N(1)—H(1)	0·82 (4)	0·77 (3)
C(2)—H(2)	0·97 (4)	0·94 (4)
C(4)—H(4)	0·96 (4)	0·99 (3)
C(6)—H(6)	1·04 (4)	1·03 (4)
C(7)—H(7)	0·95 (4)	1·01 (3)
O(10)–H(10)	0·95 (4)	0·79 (3)
C(11)–H(11*A*)	1·05 (4)	1·00 (4)
C(11)–H(11*B*)	0·97 (3)	0·93 (3)
C(12)–H(12*A*)	1·05 (3)	0·98 (4)
C(12)–H(12*B*)	1·02 (4)	0·93 (4)
C(14)–H(14*A*)	0·93 (2)	1·03 (3)
C(14)–H(14*B*)	0·95 (3)	0·99 (4)
C(14)–H(14*C*)	1·03 (4)	1·02 (5)
C(15)–H(15*A*)	1·01 (3)	1·02 (3)
C(15)–H(15*B*)	1·04 (4)	1·05 (4)
C(15)–H(15*C*)	1·00 (4)	1·02 (4)
O(10)···N(13′)	2·676 (4)	2·719 (5)
H(10)···N(13′)	1·75 (3)	1·97 (4)

From Fig. 2 it is obvious that the two bufotenine molecules are nearly identical. The differences in bond distances and angles for non-hydrogen atoms never exceed 0·02 Å and 1·9° respectively, which are close to the e.s.d.'s.

Table 6. *Bond angles and estimated standard deviations (in parentheses) for all non-hydrogen atoms*

	Molecule *A*	Molecule *B*
N(1)–C(2)–C(3)	109·5 (5)°	109·7 (5)°
C(2)–C(3)–C(9)	105·7 (5)	105·0 (5)
C(3)–C(9)–C(8)	108·6 (5)	110·5 (5)
C(9)–C(8)–N(1)	105·9 (5)	104·2 (5)
C(8)–N(1)–C(2)	110·2 (5)	110·6 (5)
C(4)–C(5)–C(6)	122·2 (5)	122·3 (5)
C(5)–C(6)–C(7)	119·4 (5)	119·0 (5)
C(6)–C(7)–C(8)	118·3 (5)	118·5 (5)
C(7)–C(8)–C(9)	123·2 (5)	123·9 (5)
C(8)–C(9)–C(4)	118·0 (5)	116·4 (5)
C(9)–C(4)–C(5)	118·9 (5)	119·7 (5)
C(4)–C(5)–O(10)	123·6 (5)	123·4 (5)
C(6)–C(5)–O(10)	114·2 (5)	114·2 (5)
N(1)–C(8)–C(7)	130·9 (5)	131·9 (5)
C(3)–C(9)–C(4)	133·4 (5)	133·1 (5)
C(2)—C(3)—C(11)	125·1 (5)	125·2 (5)
C(9)—C(3)—C(11)	129·1 (5)	129·6 (5)
C(3)—C(11)–C(12)	110·7 (4)	109·5 (4)
C(11)–C(12)–N(13)	112·8 (4)	114·7 (4)
C(12)–N(13)–C(14)	113·6 (4)	112·4 (4)
C(12)–N(13)–C(15)	108·7 (4)	108·7 (4)
C(14)–N(13)–C(15)	108·5 (4)	109·4 (4)
O(10)–H(10)···N(13′)	166·7	156·5
O(10)···N(13′)–C(12′)	101·6	102·4
O(10)···N(13′)–C(14′)	121·1	112·6
O(10)···N(13′)–C(15′)	102·2	111·3

The planarity of the indole nuclei

Least-squares planes were calculated for both molecules *A* and *B* through the indole nucleus, and for the benzene and pyrrole rings separately. Distances of atoms from these least-squares planes are shown in Table 7, in which the equations of the best planes are also given. The atoms constituting the indole ring system of molecule *A* lie on a common plane except for the nitrogen atom N(1), which deviates 0·021 Å, *i.e.* more than three standard deviations, from the plane. This is significant according to Cruickshank (1949). The angle between the benzene and pyrrole rings of molecule *A* is 0·80° and does not differ significantly from planarity. In molecule *B*, the deviations of the atoms from the indole plane are more pronounced, the mean deviation being ±0·014 Å. The mean deviations of the atoms from the benzene plane and from the pyrrole plane are ±0·010 and ±0·006 Å respectively, which shows that these rings taken separately are planar within experimental error. The angle between the two portions of the indole nucleus is 1·46°. A similar but even larger bending has been found in some indole derivatives (Bergman, Abrahamsson & Dahlén, 1971; Falkenberg & Carlström, 1971).

In molecule *A* the oxygen atom, O(10), which is attached to the benzene ring, lies in the plane of this ring. In the *B* molecule, however, O(10) departs from the benzene plane by 0·022 Å, which is more than three standard deviations. The deviation from the indole plane is even larger, 0·037 Å.

The carbon atom, C(11), connected to the pyrrole ring, deviates significantly from the indole plane in both molecules. In the *B* molecule the deviation of this atom from the pyrrole plane is as much as 0·1 Å.

Bond lengths and bond angles

The C(4)–C(5) bond, 1·361 Å (1·351 Å), in both molecules is significantly shorter than the C–C standard bond for benzene, 1·397±0·001 Å. This short-

Table 7. *Bond angles and estimated standard deviations (in parentheses) for all bonds involving hydrogen atoms*

	Molecule *A*	Molecule *B*
C(8)–N(1)—H(1)	123 (3)°	121 (3)°
C(2)–N(1)—H(1)	125 (3)	126 (3)
N(1)–C(2)—H(2)	128 (3)	132 (3)
C(3)–C(2)—H(2)	123 (3)	118 (3)
C(5)–C(4)—H(4)	120 (3)	127 (2)
C(9)–C(4)—H(4)	121 (3)	114 (2)
C(5)–O(10)–H(10)	109 (3)	103 (3)
C(5)–C(6)–H(6)	119 (2)	121 (2)
C(7)–C(6)–H(6)	122 (2)	120 (2)
C(6)–C(7)–H(7)	121 (3)	115 (2)
C(8)–C(7)–H(7)	121 (3)	126 (3)
C(3)—C(11)–H(11*A*)	113 (2)	114 (3)
C(3)—C(11)–H(11*B*)	109 (3)	105 (3)
C(12)–C(11)–H(11*A*)	106 (2)	107 (3)
C(12)–C(11)–H(11*B*)	113 (3)	116 (3)
H(7)—C(11)–H(11*B*)	105 (4)	105 (4)
C(11)—C(12)–H(12*A*)	108 (2)	115 (3)
C(11)—C(12)–H(12*B*)	108 (2)	105 (3)
N(13) —C(12)–H(12*A*)	109 (2)	104 (3)
N(13) —C(12)–H(12*B*)	108 (2)	110 (3)
H(12*A*)–C(12)–H(12*B*)	111 (3)	108 (4)
N(13) —C(14)–H(14*A*)	106 (3)	109 (3)
N(13) —C(14)–H(12*B*)	110 (3)	116 (3)
N(13) —C(14)–H(14*C*)	116 (2)	111 (3)
H(14*A*)–C(14)–H(14*B*)	112 (4)	110 (4)
H(14*A*)–C(14)–H(14*C*)	107 (4)	118 (4)
H(14*B*)–C(14)–H(14*C*)	105 (4)	94 (4)
N(13) —C(15)–H(15*A*)	117 (2)	119 (2)
N(13) —C(15)–H(15*B*)	103 (2)	102 (2)
N(13) —C(15)–H(15*C*)	108 (3)	111 (3)
H(15*A*)–C(15)–H(15*B*)	108 (3)	109 (3)
H(15*A*)–C(15)–H(15*C*)	104 (3)	99 (3)
H(15*B*)–C(15)–H(15*C*)	116 (3)	118 (3)

ening is consistent with that found in dimethyltryptamine which has no hydroxy group attached to the six-membered ring (Falkenberg, 1972). The other five bonds in the benzene ring have an average length of 1·386 ± 0·007 Å (1·390 ± 0·009 Å), which is not significantly different from the standard C–C bond for benzene.

The C(5)–O(10) bond, 1·378 Å (1·369 Å), is in good agreement with the corresponding bond in 5-hydroxytryptamine (serotonin), 1·388 ± 0·003 Å (recalculated from Thewalt & Bugg, 1972), and also close to the standard shortened single C–O bond, 1·36 ± 0·01 Å, of oxygen attached to aromatic ring systems.

In the pyrrole portion of the indole nucleus the C–N distances C(2)–N(1), 1·356 Å (1·353 Å), and C(8)–N(1), 1·366 Å (1·377 Å), are statistically equivalent. The average of these C–N bonds, 1·363 ± 0·002 Å, is not significantly different from the corresponding bonds of earlier determined indole nuclei (Falkenberg & Carlström, 1971). In both molecules *A* and *B* the C(2)–C(3) bond, 1·361 Å (1·363 Å), is shorter than the C(3)–C(9) bond, 1·422 Å (1·404 Å). These bonds have the atom C(3) in common and are thus not independent. It is however possible to compare the bonds of the two independent molecules. From this comparison it is clear that the bonds in question have statistically different lengths. A pronounced double-bond character of the C(2)–C(3) bond is thus indicated, which is consistent with earlier results (Quarles, 1971; Falkenberg & Carlström, 1971; Thewalt & Bugg, 1972; Falkenberg, 1972).

The two C–C bonds of the ethylamine chain, C(3)–C(11), 1·498 Å (1·489 Å), and C(11)–C(12), 1·514 Å (1·514 Å), are significantly shorter than the standard paraffinic single bond, 1·541 Å. The atomic distance from the α-carbon atom to the tertiary amino nitrogen, C(12)–N(13), 1·450 Å (1·461 Å), is, when tested statistically, equal to the corresponding bond in dimethyltryptamine, 1·464 Å (1·458 Å), (Falkenberg, 1972), in 5-methoxy tryptamine, 1·457 Å, and in melatonin, 1·448 Å (Quarles, 1971). All these figures refer to structures in which the amino nitrogen atom is unprotonized. The mean of the six C–N bonds around N(13) *A* and *B*, 1·462 Å, is slightly shorter than the 3-covalent C–N standard bond, 1·472 Å, and significantly shorter than the $C–N^+$ bond of 1·503 Å (Hahn, 1957). The bond angles involving N(13) are all close to the tetrahedral value, 109·5°, which is consistent with the results found for chlorpromazine (McDowell, 1969). This situation is comparable to that in ammonia, which has a lone electron pair.

Conformation of the ethylamine chain

The torsion angle τ_1 = C(2)–C(3)–C(11)–C(12) describes the position of the α-carbon atom in the ethylamine chain in relation to the ring system, $\tau_1 = 87°$ (72°). The plane defined by C(3)C(11)C(12) is thus nearly perpendicular to the plane of the indole nucleus. The ethylamine chain is almost maximally extended (Fig. 2) and the torsion angle τ_2 = C(3)–C(11)–C(12)–N(13) is 175° (170°). The conformation of the side chain gives a staggered arrangement with the carbon atom C(15), belonging to one of the methyl groups, in an *anti*-periplanar position relative to the α-carbon, C(12). The carbon atom C(14) of the second methyl group is *syn*-clinal relative to C(12), (Fig. 2).

Arrangement of the hydrogen atoms

The accuracy in the determination of the hydrogen positions is somewhat lower than that indicated by the e.s.d.'s. There are minor distortions in the molecular geometry due to the unreliability of the hydrogen coordinates. In the methyl groups the bond angles deviate considerably from the tetrahedral value (Table 7). Among the hydrogen atoms attached to the ring system, there are sizable deviations from the indole plane. In molecule *A* the deviations of the five hydrogen atoms in question range from +0·13 to −0·13 Å and in molecule *B* they range from +0·08 to −0·15 Å. These figures should be compared with the small deviations of the non-hydrogen atoms from the best planes (Table 4). The C–H bond lengths of molecules *A* and *B* are in the same range, 0·93–1·05 Å, with a mean value of 1·0 Å, which is in good agreement with the standard C–H bond of 1·1 Å. The N–H bond, 0·82 Å (0·77 Å), is shorter than the standard length of 0·93 Å. In molecule *A*, the O–H bond, 0·95 Å, is quite acceptable, while the corresponding bond in molecule *B*, 0·79 Å, is slightly shorter than the standard bond 0·97 Å. The angular geometry of the hydrogen atoms (Table 6) is consistent with earlier works (Quarles, 1971; Falkenberg & Carlström, 1971). There are no significant differences between the bond angles in molecules *A* and *B*.

Hydrogen bonds and packing of the molecules

The crystal structure viewed along the *c* axis is given in Fig. 3. The *A*-molecules are linked by hydrogen bonds, O(10)–H(10)···N(13), which run in a helical fashion around a screw axis. The hydrogen bonding system for the *B*-molecules has similar arrangement. The O···N distance, 2·68 Å (2·72 Å), is in good agreement with the O–H···N hydrogen bond found in dimethylglyoxime, 2·766 ± 0·020 Å (Hamilton, 1961). The O···N bond forms almost tetrahedral angles with the carbon atoms around the acceptor atom N(13) (Table 6), and the hydrogen atom H(10) is directed towards the lone electron pair of the amino nitrogen atom. The hydrogen bonds are thus almost linear, 166·7° (156·5°). The shortest intermolecular distance for non-hydrogen atoms is 3·548 Å. The connexions between the *A*- and *B*-molecules are ordinary van der Waals contacts.

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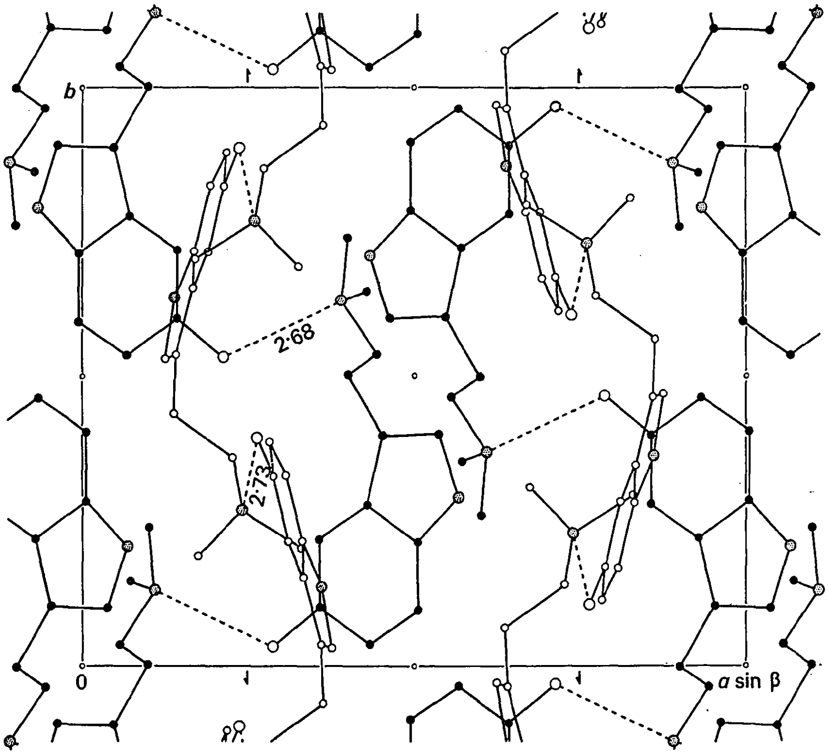

Fig. 3. Molecular packing in bufotenine viewed along the *c* axis. Carbon atoms are represented by full and open small circles, indicating atoms of molecules *A* and *B* respectively. Larger dotted and open circles represent nitrogen and oxygen atoms respectively. Hydrogen bonds are dashed and the distances are given in Å.

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Etudes Cristallographiques en Série Sesquiterpénique. III. Structure Cristalline et Moléculaire du Bromo-7 Cyclo[3:15]longifolane

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The molecular structure and absolute configuration of 7-bromocyclo[3:15]longifolane, $C_{15}H_{23}Br$, have been established by a three-dimensional single-crystal X-ray analysis. The crystals are orthorhombic, space group $P2_12_12_1$ and the cell constants are: $a=20\cdot53\pm0\cdot02$, $b=6\cdot901\pm0\cdot007$, $c=9\cdot251\pm0\cdot009$ Å, with $Z=4$. The structure was solved by the heavy-atom method and refined by least-squares techniques to $R=0\cdot043$ for 748 independent reflexions measured by diffractometry. The absolute configuration was established taking into account the anomalous dispersion effect from bromine atoms. The geometry of a new adamantane-type tetracyclic sesquiterpene skeleton is described.

Introduction

La détermination de la structure cristalline et moléculaire du bromo-7 cyclo[3:15]longifolane a été entreprise dans le cadre de l'étude par rayons X des réactions transannulaires du longifolène. Helmlinger & Ourisson (1969) ont obtenu, par isomérisation du bromo-3α longifolène, un dérivé tétracyclique nouveau, issu d'une cyclisation transannulaire, pour lequel l'hypothèse de structure déduite de ses réactions (Fig. 1) a été prouvée par cette étude radiocristallographique. Un article préliminaire relatif à cette structure a déjà été publié (Thierry & Weiss, 1969). Nous donnons ici les détails de l'étude par rayons X de ce nouveau dérivé tétracyclique de type adamantoïde.

Partie expérimentale

Les monocristaux nécessaires à la détermination de la structure du bromo-7 cyclo[3:15]longifolane ont été obtenus par recristallisation lente dans l'acétate d'éthyle. Ils se présentent sous forme d'aiguilles dont l'axe d'allongement est orienté selon [010]. La classe de Laue, le groupe d'espace et les paramètres ont été déterminés à partir de clichés de diffraction effectués sur une chambre de précession, préalablement étalonnée à l'aide d'un monocristal de chlorure de sodium, avec le rayonnement $K\bar{\alpha}$ du cuivre. Les extinctions systématiques ($h00$ avec $h=2n+1$, $0k0$ avec $k=2n+1$, $00l$ avec $l=2n+1$) conduisent sans ambiguïté au groupe spatial $P2_12_12_1$ seul compatible avec l'activité optique du dérivé $[\alpha]_D=66°$. La densité (D_m) a été mesurée par flottaison dans une solution aqueuse d'iodure de potassium.

Données cristallines

$C_{15}H_{23}Br$, $M=283{,}3$, orthorhombique; $a=20{,}53\pm0{,}02$, $b=6{,}901\pm0{,}007$, $c=9{,}251\pm0{,}009$ Å; $U=1311$ Å^3 $D_m=1{,}42\pm0{,}02$, $Z=4$, $D_c=1{,}437$; $F(000)=592$, $\mu=31{,}1$ cm^{-1} pour $K\bar{\alpha}$ du cuivre (λ moyen $=1{,}54178$ Å), groupe spatial $P2_12_12_1$ (D_2^4, No. 19).

La mesure des intensités diffractées a été réalisée à l'aide d'un diffractomètre automatique à monocristal Philips PAILRED, à la longueur d'onde du cuivre ($\lambda K\bar{\alpha}$) en utilisant le plan réflecteur (111) d'une lame