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Structure of 3-Isoinosine

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Abstract. 3-β-D-Ribofuranosylhypoxanthine, 3-β-D-ribofuranosyl-1,6-dihydro-3*H*-purin-6-one, $C_{10}H_{12}N_4O_5$, $M_r = 268·23$, monoclinic, $P2_1$, $a = 6·503\ (1)$, $b = 24·007\ (6)$, $c = 7·392\ (2)$ Å, $\beta = 106·53\ (2)°$, $V = 1106·3\ (9)$ Å^3, $Z = 4$, $D_x = 1·610$ g cm^{-3}, λ(Mo $K\bar{\alpha}$) = 0·71073 Å, $\mu = 1·23$ cm^{-1}, $F(000) = 560$, $T = 299$ K, $R = 0·048$ and $wR = 0·043$ for 1602 observed reflections. There are two crystallographically independent molecules in the structure; in both of them the 6-oxo, 7*H* tautomer is the predominant form. The bond lengths and angles of the two molecules are almost identical and the hypoxanthine moiety is almost planar. The torsional angles of the glycosidic linkage O(4′)—C(1′)—N(3)—C(4) are −159·3 and −148·8°, both in the *anti* range. The sugar puckers are $_4T^3$ (C4′-*exo*/C3′-*endo*), with $P = 46·35°$ and $\tau_m = 42·30°$, and ^2E (C2′-*endo*), with $P = 157·24°$ and $\tau_m = 41·32°$. All N and O atoms except N(3) and O(4′) participate in a three-dimensional hydrogen-bonding system.

Introduction. 3-Isoinosine (Wolfenden, Sharpless, Ragade & Leonard, 1966; Tindall, Robins, Tolman & Hutzenlaub, 1972) is an isomer of inosine in which the D-ribofuranosyl moiety is attached to N(3) of hypoxanthine. Inosine is a minor constituent of the transfer RNA's and it has been suggested (Crick, 1966; Woese, 1967) that it can form base pairs with any of the bases adenine, uracil, or cytosine. Similar to inosine, 3-isoinosine can form hydrogen bonds with any of these bases but the base pairing would be of the Hoogsteen type. Recently, we have shown that 3-isoadenosine, which is an isomer of adenosine, can form Hoogsteen-type base-pairing with uridine (Hill, Kumar, Leonard & Orgel, 1988). The X-ray structure determination of 3-isoinosine is desired in order to furnish information concerning the preferred tautomeric form in the crystal, the orientation of the ribose ring, and the intermolecular hydrogen-bonding pattern, and to compare its structure with that of inosine (Munns & Tollin, 1970; Thewalt, Bugg & Marsh, 1970).

Experimental. Crystals of 3-isoinosine, suitable for X-ray investigations, were grown from 70% ethanol–water at room temperature. A transparent, colorless, plate-like crystal approximately 0·1 × 0·3 × 0·4 mm was used for data collection on an Enraf–Nonius CAD-4 automated κ-axis diffractometer with graphite-monochromatized Mo $K\bar{\alpha}$ radiation. D_m was not measured. The lattice parameters were refined using 25 reflections with 2θ values between 16·3 and 23·7°; 2214 unique reflections were measured ($-h$, $-k$, $\pm l$) to the limit of $2\theta < 52·0°$ (internal consistency, $R_{\rm int} = 0·016$) using the ω/θ-scan technique, scan rate 2·0–8·0° min^{-1}, scan width $(1·00 + 0·35\tan\theta)°$ with a scan to background ratio of 0·33, 1602 reflections with $I > 2·58\sigma(I)$, $\sigma(F_o^2)$ based on counting statistics plus the term $0·02F_o^2$. The data were corrected numerically (Busing & Levy, 1957) for absorption (max. and min. transmission factors, 0·978 and 0·958), and anomalous-dispersion, Lorentz and polarization corrections were applied. Three standard intensities monitored per 2700 s exposure time showed no significant intensity variation. The structure was solved using the direct-methods program *SHELX*86 (Sheldrick, 1985). The correct positions for all non-H atoms were deduced from an *E* map and independently refined [*SHELX*76 (Sheldrick, 1976)]. In the final cycle of least squares, all C atoms were refined with isotropic thermal coefficients and all the remaining non-H atoms were refined with anisotropic thermal coefficients in a full-matrix process that minimized $\sum[w(|F_o| - |F_c|)^2]$, where $w = 1/[\sigma(F_o)]^2$. The atomic scattering factors, dispersion corrections and mass attenuation coefficients used were taken from *International Tables for X-ray Crystallography* (1974). H atoms were located by difference electron-density maps and were refined with a group isotropic thermal parameter, and an empirical isotropic extinction parameter converged to $7·1\ (8) \times 10^{-7}$. The final agreement factors for 1602 reflections were $R = 0·048$ and $wR = 0·043$ and goodness-of-fit $E = 1·89$; max. $|\Delta/\sigma|$ for non-H atoms $< 0·05$; range of residual electron density $+0·35$ to $-0·27$ e Å^{-3}.

Discussion. *ORTEP* views (Johnson, 1965) of the two independent molecules *A* and *B* of 3-isoinosine, together with the standard atom numbering, are given in Fig. 1. The final atomic coordinates for the non-H atoms are given in Table 1, and selected bond

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lengths and bond angles are listed in Table 2.* As has been found for inosine, 3-isoinosine exists in the 6-oxo form. Within the base moiety of each independent 3-isoinosine molecule, the differences in the bond lengths and angles are less than 0·03 Å [except N(7)—C(8), 0·035 Å] and 0·6°. The largest differences between analogous bond angles occur in the ribose moieties [C(1′)—C(2′)—O(2′), 7·7° and C(3′)—C(4′)—C(5′), 4·3°] and may be attributed to the differences in the number of hydrogen bonds formed by O(2′) in molecules *A* (two) and *B* (one). When compared with those in hypoxanthine (Schmalle, Hänggi & Dubler, 1988) and inosine (Munns & Tollin, 1970; Thewalt *et al.*, 1970), the bond lengths in 3-isoisosine are similar but the bond angles in the base moiety are different. The largest differences between the bond angles in the base moieties of inosine (Thewalt *et al.*, 1970) and 3-isoinosine involve the C(4)—C(5) vector [N(3)—C(4)—C(5), 8·4°; N(9)—C(4)—C(5), 7·6°; C(4)—C(5)—C(6), 4·0°; and C(4)—C(5)—N(7), 6·5°]. The N(3)—C(1′) bond length, 1·490 (9) Å, in 3-isoinosine is similar to

Table 1. *Final atomic parameters for non-*H *atoms with e.s.d.'s in parentheses and isotropic thermal parameters*

	x	*y*	*z*	U_{iso}(Å^2)
N(1*A*)	0·2778 (8)	0·1075	0·5951 (7)	0·041 (3)*
C(2*A*)	0·2442 (10)	0·1513 (3)	0·4854 (8)	0·034 (1)
N(3*A*)	0·1063 (7)	0·1929 (3)	0·4869 (6)	0·027 (2)*
C(4*A*)	−0·0082 (9)	0·1888 (3)	0·6181 (7)	0·024 (1)
C(5*A*)	0·0196 (9)	0·1432 (3)	0·7326 (7)	0·024 (1)
C(6*A*)	0·168 (1)	0·0996 (3)	0·7306 (8)	0·035 (2)
O(6*A*)	0·1969 (8)	0·0582 (3)	0·8340 (7)	0·056 (3)*
N(7*A*)	−0·1127 (8)	0·1527 (3)	0·8454 (7)	0·033 (3)*
C(8*A*)	−0·2049 (10)	0·2019 (3)	0·7966 (9)	0·034 (1)
N(9*A*)	−0·1447 (7)	0·2269 (3)	0·6561 (7)	0·033 (3)*
C(1′*A*)	0·0697 (9)	0·2421 (3)	0·3587 (7)	0·025 (1)
C(2′*A*)	0·1977 (9)	0·2929 (3)	0·4484 (8)	0·028 (1)
O(2′*A*)	0·0520 (6)	0·3397 (2)	0·4141 (6)	0·046 (2)*
C(3′*A*)	0·3615 (10)	0·2993 (3)	0·3393 (8)	0·028 (1)
O(3′*A*)	0·4212 (7)	0·3553 (2)	0·3240 (6)	0·043 (3)*
C(4′*A*)	0·2444 (9)	0·2753 (3)	0·1500 (8)	0·026 (1)
O(4′*A*)	0·1409 (6)	0·2269 (2)	0·2013 (5)	0·033 (2)*
C(5′*A*)	0·379 (1)	0·2584 (3)	0·0233 (9)	0·031 (1)
O(5′*A*)	0·5740 (7)	0·2334 (3)	0·1143 (6)	0·045 (3)*
N(1*B*)	−0·1668 (8)	0·0826 (3)	0·1442 (7)	0·038 (3)*
C(2*B*)	−0·0425 (9)	0·0390 (3)	0·1593 (8)	0·032 (1)
N(3*B*)	−0·0268 (8)	−0·0031 (3)	0·2830 (6)	0·030 (2)*
C(4*B*)	−0·1505 (9)	0·0007 (3)	0·4051 (8)	0·028 (1)
C(5*B*)	−0·2796 (9)	0·0459 (3)	0·3963 (8)	0·027 (1)
C(6*B*)	−0·3012 (10)	0·0896 (3)	0·2614 (8)	0·036 (1)
O(6*B*)	−0·4189 (8)	0·1300 (3)	0·2488 (7)	0·063 (3)*
N(7*B*)	−0·3774 (8)	0·0372 (3)	0·5355 (7)	0·038 (3)*
C(8*B*)	−0·3043 (9)	−0·0125 (3)	0·6173 (8)	0·034 (1)
N(9*B*)	−0·1630 (8)	−0·0367 (3)	0·5416 (6)	0·033 (2)*
C(1′*B*)	0·1150 (9)	−0·0521 (3)	0·2916 (8)	0·025 (1)
C(2′*B*)	0·0188 (9)	−0·0988 (3)	0·1558 (7)	0·025 (1)
O(2′*B*)	−0·1326 (6)	−0·1325 (2)	0·2105 (6)	0·035 (2)*
C(3′*B*)	0·2201 (9)	−0·1285 (3)	0·1461 (8)	0·026 (1)
O(3′*B*)	0·3046 (6)	−0·1617 (3)	0·3119 (6)	0·038 (2)*
C(4′*B*)	0·3734 (9)	−0·0807 (3)	0·1498 (8)	0·029 (1)
O(4′*B*)	0·2930 (6)	−0·0340 (2)	0·2373 (5)	0·036 (2)*
C(5′*B*)	0·380 (1)	−0·0640 (3)	−0·0439 (9)	0·044 (2)
O(5′*B*)	0·5134 (8)	−0·0180 (3)	−0·0391 (7)	0·058 (3)*

* Equivalent isotropic *U* is defined as one-third the value of the orthogonalized U_{ij} tensor.

Table 2. *Selected bond lengths* (Å) *and bond angles* (°)

	A	*B*		*A*	*B*
N(1)—C(2)	1·306 (7)	1·307 (9)	C(2)—N(3)	1·346 (9)	1·347 (9)
N(3)—C(4)	1·384 (7)	1·372 (7)	C(4)—C(5)	1·365 (9)	1·361 (9)
N(1)—C(6)	1·398 (8)	1·404 (8)	C(5)—C(6)	1·427 (9)	1·427 (9)
C(6)—O(6)	1·236 (9)	1·223 (9)	C(5)—N(7)	1·377 (7)	1·371 (7)
N(7)—C(8)	1·327 (9)	1·362 (9)	C(4)—N(9)	1·359 (8)	1·370 (8)
C(8)—N(9)	1·351 (8)	1·337 (8)	N(3)—C(1′)	1·490 (9)	1·485 (9)
C(1′)—C(2′)	1·519 (9)	1·515 (9)	C(2′)—O(2′)	1·444 (8)	1·419 (7)
C(2′)—C(3′)	1·516 (8)	1·511 (8)	C(3′)—O(3′)	1·414 (9)	1·433 (7)
C(3′)—C(4′)	1·504 (8)	1·517 (9)	C(1′)—O(4′)	1·418 (7)	1·398 (7)
C(4′)—O(4′)	1·448 (8)	1·464 (8)	C(4′)—C(5′)	1·509 (9)	1·498 (9)
C(5′)—O(5′)	1·390 (8)	1·401 (10)	C(2)—N(1)—C(6)	121.6 (5)	121·4 (6)
N(1)—C(2)—N(3)	125·9 (5)	125·7 (5)	C(2)—N(3)—C(4)	116·4 (6)	116·8 (6)
C(2)—N(3)—C(1′)	124·8 (5)	123·4 (5)	C(4)—N(3)—C(1′)	118·8 (5)	119·9 (5)
N(3)—C(4)—C(5)	119·3 (6)	119·4 (6)	N(3)—C(4)—N(9)	127·6 (6)	127·5 (6)
C(5)—C(4)—N(9)	113·0 (5)	113·0 (5)	C(4)—C(5)—C(6)	123·5 (5)	123·7 (5)
C(4)—C(5)—N(7)	104·3 (5)	104·8 (5)	C(6)—C(5)—N(7)	132·0 (6)	131·4 (6)
N(1)—C(6)—C(5)	113·1 (5)	112·9 (6)	N(1)—C(6)—O(6)	122·3 (6)	122·3 (6)
C(5)—C(6)—O(6)	124·5 (6)	124·9 (6)	C(5)—N(7)—C(8)	107·1 (5)	106·7 (5)
N(7)—C(8)—N(9)	113·4 (6)	112·9 (5)	C(4)—N(9)—C(8)	102·1 (6)	102·5 (6)
N(3)—C(1′)—C(2′)	113·0 (4)	115·0 (5)	N(3)—C(1′)—O(4′)	106·6 (5)	107·2 (5)
C(2′)—C(1′)—O(4′)	107·5 (5)	105·1 (5)	C(1′)—C(2′)—O(2′)	107·3 (5)	115·0 (5)
C(1′)—C(2′)—C(3′)	103·2 (5)	100·4 (4)	O(2′)—C(2′)—C(3′)	110·7 (5)	115·1 (5)
C(2′)—C(3′)—O(3′)	112·8 (5)	110·4 (4)	C(2′)—C(3′)—C(4′)	102·1 (5)	102·4 (5)
O(3′)—C(3′)—C(4′)	111·5 (5)	108·4 (4)	C(3′)—C(4′)—O(4′)	102·3 (5)	105·8 (5)
C(3′)—C(4′)—C(5′)	116·8 (5)	112·5 (5)	O(4)—C(4)—C(5′)	109·9 (6)	109·2 (6)
C(1′)—O(4′)—C(4′)	107·0 (5)	108·5 (5)	C(4′)—C(5′)—O(5′)	115·2 (5)	111·8 (6)

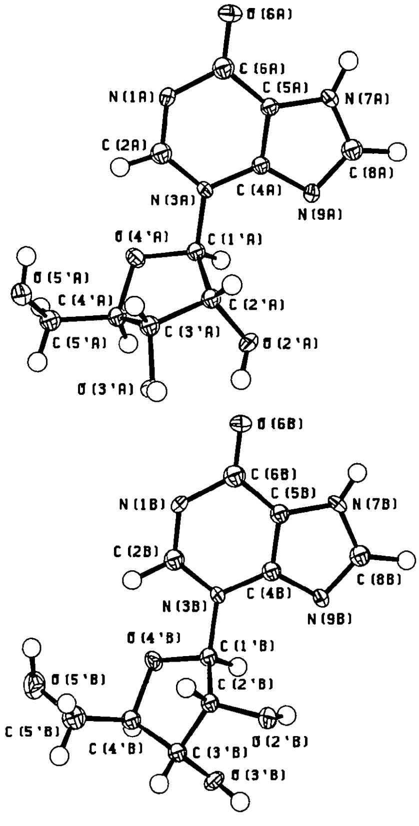

Fig. 1. An *ORTEP* drawing (Johnson, 1965), with the atom numbering, of two independent molecules of 3-isoinosine in the crystal.

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* Lists of refined H-atom coordinates, anisotropic thermal parameters, torsion angles, observed and calculated structure-factor amplitudes, deviations from the hypoxanthine plane, and a stereo figure of the unit cell have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 51886 (15 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

that in 3-isoadenosine (1·488 Å) (Kumar, Wilson & Leonard, 1988) and is comparable to that in inosine [N(9)—C(1′), 1·477 Å] and inosine dihydrate (1·452 Å) (Thewalt *et al.*, 1970).

The hypoxanthine ring in both molecules is nearly planar (Fig. 1) but is slightly folded about the C(4)—C(5) vector with interplanar angles of 3·3 and 1·1°, respectively. The largest deviation from the least-squares planes of the base moieties in *A* and *B* is 0·036 (6) Å for atom C(5) in molecule *A*. In inosine, the sugar has the C(3′)-*endo* conformation (Munns & Tollin, 1970) whereas in inosine dihydrate, it is C(2′)-*endo* in both the molecules (Thewalt *et al.*, 1970). In 3-isoinosine, the sugar torsional angles ν_0 through ν_4 [*i.e.* those for the ring bonds O(4′)—C(1′), C(1′)—C(2′) and clockwise around the ring] are −20·2 (6), −6·5 (6), 29·2 (6), −41·6 (6), 38·9 (6), and −27·9 (6), 41·4 (6), −38·1 (5), 23·0 (6), 2·9 (6)° for molecules *A* and *B*, respectively; the corresponding pseudorotational angles (*P*) calculated from these torsional angles are 46·35 and 157·24°, which indicates that the sugar conformation is $_4T^3$ (C4′-*exo*/C3′-*endo*) in molecule *A* and ^2E (C2′-*endo*) in molecule *B*. The degrees of pucker (τ_m), as defined by Altona & Sundralingam (1972), are 42·30 and 41·32° in molecules *A* and *B*, respectively. The torsion angles about the glycosidic bond O(4′)—C(1′)—N(3)—C(4), are −159·3 and −148·8°, which indicates that both the molecules have the *anti* conformation of base relative to the sugar.

The conformation around the C(4′)—C(5′) bond, described by the angles φ_{OO} [the angle between the projected C(5′)—O(5′) and C(4′)—O(4′)] and φ_{OC} [the angle between the projected C(5′)—O(5′) and C(4′)—C(3′)] (Shefter & Trueblood, 1965) is *gauche–gauche* for both nucleosides in the inosine dihydrate and *gauche–trans* for inosine. In 3-isoinosine, the conformation around this bond is *gauche–gauche* in molecule *A*, *i.e.* C(5′)—O(5′) is *gauche* to C(4′)—O(4′) [$\varphi_{OO} = -77·0\ (7)°$] and *gauche* to C(4′)—C(3′) [$\varphi_{OC} = 38·9\ (8)°$] but in molecule *B*, it is *gauche–trans*, *i.e.* C(5′)—O(5′) is *gauche* to C(4′)—O(4′) [$\varphi_{OO} = 59·7\ (7)°$] and *trans* to C(4′)—C(3′) [$\varphi_{OC} = 176·9\ (5)°$].

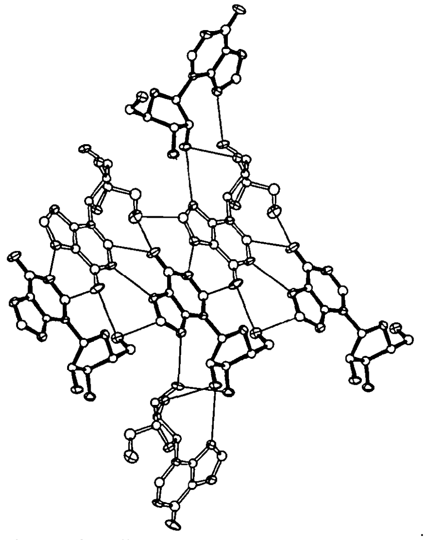

Fig. 2. Hydrogen-bonding scheme of 3-isoinosine. Hydrogen bonds are shown by thin lines.

Table 3. *Intermolecular hydrogen interactions*

	Distances (Å)			Angle (°)	Equivalent
X···H—*Y*	*X*···*Y*	*X*···H	H—*Y*	*X*···H—*Y*	position *X*
O(5′*A*)···H(8*A*)—C(8*A*)	3·174 (8)	2·20 (3)	1·09 (3)	148 (3)	$x-1, y, z+1$
O(5′*B*)···H(8*B*)—C(8*B*)	3·097 (7)	2·07 (3)	1·13 (4)	149 (4)	$x-1, y, z+1$
O(6*B*)···H(2*A*)—C(2*A*)	3·209 (8)	2·30 (3)	0·97 (3)	155 (3)	$x+1, y, z$
O(6*A*)···H(2*B*)—C(2*B*)	3·248 (7)	2·24 (3)	1·07 (3)	158 (4)	$x, y, z-1$
O(6*B*)···H(5*A*′)—O(5′*A*)	2·669 (8)	1·84 (5)	0·84 (5)	168 (4)	$x+1, y, z$
O(6*A*)···H(5*B*′)—O(5′*B*)	2·713 (8)	1·56 (4)	1·19 (4)	162 (3)	$x, y, z-1$
N(1*B*)···H(7*A*)—N(7*A*)	2·877 (8)	1·95 (4)	0·94 (4)	172 (4)	$x, y, z+1$
N(1*A*)···H(7*B*)—N(7*B*)	2·938 (7)	2·08 (4)	0·86 (4)	173 (3)	$x-1, y, z$
N(9*B*)···H(2*A*′)—O(2′*A*)	3·050 (9)	2·28 (5)	0·90 (5)	144 (3)	$-x, y+\frac{1}{2}, 1-z$
N(9*A*)···H(3*B*′)—O(3′*B*)	2·903 (8)	2·09 (5)	0·87 (5)	156 (3)	$-x, y-\frac{1}{2}, 1-z$
O(2′*A*)···H(2*B*′)—O(2′*B*)	2·756 (6)	2·00 (4)	0·80 (3)	157 (5)	$-x, y-\frac{1}{2}, 1-z$
O(3′*B*)···H(3*A*′)—O(3′*A*)	2·803 (6)	1·99 (4)	0·92 (3)	145 (4)	$1-x, y+\frac{1}{2}, 1-z$

Fig. 2 shows the hydrogen-bonding pattern in 3-isoinosine. Like inosine (Munns & Tollin, 1970) the structure of 3-isoinosine is very tightly hydrogen bonded, which accounts for the high calculated density (1·610 g cm^{-3}) and the low overall thermal motion. All of the N and O atoms except N(3) and O(4′) of 3-isoinosine participate in an extensive hydrogen-bonding scheme. The hydrogen-bond distances and angles are given in Table 3. A weak hydrogen bond, H(8*A*)···O(5′*A*), forms a side chain of *A* molecules roughly parallel to the *ac* diagonal. Likewise, another weak interaction, H(8*B*)···O(5′*B*), forms a chain of *B* molecules parallel to the *A* chain. Six hydrogen bonds link chains *A* and *B* into a ribbon with the hypoxanthine moieties along the center. This ribbon is linked to the adjacent ribbon at a dihedral angle of 60° forming a folded sheet normal to the *b* axis. One hydrogen bond, H(3′*A*)···O(3′*B*), roughly parallel to the *ac* diagonal, interlinks these folded sheets.

The 7*H* tautomer of 3-isoinosine (Fig. 1) would support Hoogsteen but not Watson–Crick base-pairing with a complementary base.

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Structures of Two Dimers Obtained by Hydrogenation of the Methyl and Trimethyl Derivatives of Hydroxyflavylium Chloride

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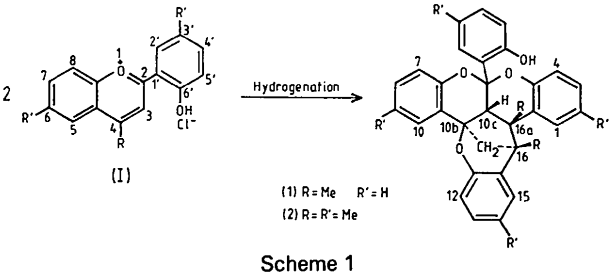
Abstract. (1) 2-[4b,5,10a,15b-Tetrahydro-5,10a-methano-4b,5-dimethyl-5a*H*-di[1](benzopyrano)-[4,3-*b*:3′,4′-*c*;2,3:2′,3′][1]benzoxepin-15a-yl]phenol acetone solvate, $C_{32}H_{26}O_4.C_3H_6O$, $M_r = 532{\cdot}64$, triclinic, $P\bar{1}$, $a = 10{\cdot}104\,(8)$, $b = 10{\cdot}981\,(7)$, $c = 14{\cdot}437\,(7)$ Å, $\alpha = 91{\cdot}76\,(4)$, $\beta = 106{\cdot}21\,(3)$, $\gamma = 110{\cdot}62\,(4)°$, $V = 1424{\cdot}7$ Å^3, $Z = 2$, $D_x = 1{\cdot}24$ g cm^{-3}, $\lambda(\text{Mo } K\alpha) = 0{\cdot}71073$ Å, $\mu = 0{\cdot}77$ cm^{-1}, $F(000) = 564$, $T = 293$ K, $R = 0{\cdot}054$ based on 2828 observed reflections with $I \geq 3\sigma(I)$. (2) 4-Methyl-[4b,5,10a,15b-tetrahydro-5,-10a-methano-3,4b,5,7,12-pentamethyl-5a*H*-di[1]-(benzopyrano)[4,3-*b*:3′,4′-*c*,-2,3:2′,3′][1]benzoxepin-5a-yl]phenol ethyl acetate solvate, $C_{36}H_{34}O_4.C_4H_8O_2$, $M_r = 618{\cdot}78$, monoclinic, $P2_1/c$, $a = 10{\cdot}10{\cdot}551\,(6)$, $b = 19{\cdot}881\,(4)$, $c = 16{\cdot}446\,(8)$ Å, $\beta = 104{\cdot}49\,(5)°$, $V = 3339{\cdot}9$ Å^3, $Z = 4$, $D_x = 1{\cdot}23$ g cm^{-3}, $\lambda(\text{Mo } K\alpha) = 0{\cdot}71073$ Å, $\mu = 0{\cdot}76$ cm^{-1}, $F(000) = 1320$, $T = 293$ K, $R = 0{\cdot}050$ based on 2994 observed reflections with $I \geq 3\sigma(I)$. The compounds are formed by the association of two flavane skeletons. This association is established at three points (C7⋯C18, O3⋯C16 and C9⋯C17) and results in the formation of a five-membered ring and a heterocycle. All the junction C atoms are sp^3 hybridized and the molecules are not planar.

Introduction. Few examples of the reduction of flavylium salts have appeared in the literature (Reynolds, Van Allan & Regan, 1967; Reynolds & Van Allan, 1967; Jurd & Roitman, 1978). These structures are assigned on the basis of the NMR, IR and mass spectra. We have reported recently a procedure used for the reduction of 2′-hydroxy-4′-methylflavylium chloride and its 4,6,3′-trimethyl derivative (I) which results in the formation of (1) and (2) (Scheme 1) (Jolibois, Vebrel, Ouahab, Boultif & Grandjean, 1988).



Scheme 1

The molecular structures consist of two associated flavane skeletons (I) and we deemed it necessary to determine precisely the junction points of this association. The inductive effect of supplementary methyl groups could induce a different type of linkage. We therefore determined the structures of compounds (1) and (2).

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