The shortest packing contacts in the crystal involve the N atoms, namely N$\cdots$N($\bar{x}$, 1$-y$, $-1-z$) 3·24 (1), N$\cdots$S(x, y, $z-1$) 3·201 (4), N$\cdots$H$_2$—C$_2$($\frac{1}{2}-x$, $\frac{1}{2}+y$, $-\frac{1}{2}-z$) 2·56 (3) Å. The last contact, already found in 4,4′-dimethyl-2,2′-bithiazole (Bolognesi *et al.*, 1987), constitutes evidence for hydrogen-bond formation between the N and C atoms [see for confirmation the range of hydrogen-bond distances (2·3–2·6 Å) in Taylor & Kennard (1982)]. Finally one can infer that H2 has some acidic character, as found in bithiazole derivatives (Bolognesi *et al.*, 1987).

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The Structure of 1,6-Dihydroxy-7,8-dimethoxyxanthone

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Abstract. C$_{15}$H$_{12}$O$_6$, $M_r = 288·3$, monoclinic, $A2/a$, $a = 14·081$ (4), $b = 12·397$ (4), $c = 16·335$ (5) Å, $\beta = 116·38$ (7)°, $V = 2554$ (1) Å^3, $Z = 8$, $D_m = 1·48$ (3), $D_x = 1·50$ Mg m^{-3}, λ(Co $K\alpha$) = 1·7903 Å, $\mu = 1·55$ mm^{-1}, $F(000) = 1200$, $T = 298$ K, $R = 0·078$, $wR = 0·076$ for 1250 independent reflections. The xanthone ring is roughly planar with normal bond lengths and angles, and the molecules in the crystal are stabilized by O—H$\cdots$O type hydrogen bonds. The planes of the xanthone rings are stacked alternately at distances of 3·50 (3) and 5·80 (3) Å.

Introduction. Xanthones are heterocyclic ring systems that have many pharmacological applications. The title compound was supplied by Dr Gopalakrishna of Government Medical Stores, Madras. The present work was undertaken to study the effect of substituents on the conformation of the xanthone system.

Experimental. D_m by flotation; yellow needles (from methanol) 0·3 × 0·5 × 0·3 mm; Picker four-circle manual diffractometer (at the Department of Crystallography and Biophysics, University of Madras); $\theta/2\theta$ scan technique; Co $K\alpha$ radiation. Cell parameters refined from 34 strong accurately centred reflections in the range $30 \leq 2\theta \leq 58°$; Lp correction, absorption ignored; 1402 unique reflections with $2\theta \leq 130°$ and with $0 \leq h \leq 14$, $0 \leq k \leq 12$, $-16 \leq l \leq 14$; 1250 observed reflections with $|F_o| > 3·0\sigma(|F_o|)$; solution using *MULTAN*80 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980); two standard reflections monitored for every 100 reflections; $|E| \geq 1·30$ for phase generation, E map revealed all non-H atoms except C atom of the methoxy group at position 7 whose position and all H-atom positions were subsequently located from $\Delta\rho$ map. Full-matrix refinement (Gantzel, Sparks & Trueblood, 1961); anisotropic temperature factors for non-H atoms and isotropic for H atoms. The function minimized was $\sum w(F_o - F_c)^2$, where $w = 1/|F_o|^2$ if $|F_o| \geq |F_o|_{min}$ and $w = 1/|F_o|_{min}^2$ if $F_o < |F_o|_{min}$ with $|F_o|_{min} = 15·0$; max. $(\Delta/\sigma) = 0·3$; final

$R(F) = 0.078$ and $wR(F) = 0.076$. The relatively large R values are probably due to uncorrected absorption effects resulting from the use of Co $K\alpha$ radiation. The final difference synthesis showed no peaks either positive or negative exceeding 0.34 e Å^{-3}. All scattering factors for non-H atoms from *International Tables for X-ray Crystallography* (1962), for H atoms from Stewart, Davidson & Simpson (1965).* All calculations were performed using the IBM 1130 computer at the University of Madras and the IBM 370 computer at the Indian Institute of Technology, Madras.

Discussion. Atomic positions and the equivalent isotropic temperature factors are listed in Table 1 and an ORTEP plot (Johnson, 1965) of the molecule with the numbering scheme is shown in Fig. 1.

The bond lengths and angles in the structure are normal and similar to those observed in other pyronoid structures (Stout, Stout & Welsh, 1963; Stout, Lin & Singh, 1969; Smith & Duax, 1975; Fukuyama, Tsukihara, Kishida, Katsube, Ishida, Hamasaki & Hatsuda, 1975; Fukuyama, Hamada, Tsukihara, Katsube, Hamasaki & Hatsuda, 1976; Fukuyama, Hamada, Tsukihara & Katsube, 1978; Schmalle, Jarchow, Hausen & Schulz, 1982; Biswas & Sen, 1982; Vijayalakshmi, Rajan, Srinivasan & Ramachandran Nair, 1986).

The xanthone ring as a whole is roughly planar $[\sum(\Delta/\sigma)^2 = 490]$ and the rings A, B and C are individually planar $[\sum(\Delta/\sigma)^2 = 38$, 14 and 52 respectively]. Rings A, B and C are inclined at angles of less than $3°$ to one another. The methoxy planes formed by C(7), O(5), C(14) and C(8), O(6) C(15) are rotated through 66.3 (5) and 68.3 (6)° respectively from the plane of the xanthone ring so that C(14) and C(15) are well out of the plane of the xanthone ring system. Thus the overlap of the unshared electrons of O(5) and O(6) with the aromatic π cloud is minimal and the angles C(7)—C(8)—O(6) and C(6)—C(7)—O(5) are close to $120°$ (Stout, Lin & Singh, 1969).

The molecular packing is shown in Fig. 2 in a stereoview down the b axis with $5°$ rotation around the plotter z axis using the program of Radhakrishnan (1982). The molecules form parallel planes similar to those observed in other xanthones (Soderholm, Sonnerstam, Norrestam & Palm, 1976; Fukuyama, Hamada, Tsukihara & Katsube, 1978). The xanthone ring plane at $-x + 2$, $-y$, $-z + 2$ is at a distance of 3.50 (3) Å and that at $-x + 2$, $-y + 1$, $-z + 2$ is

5.80 (3) Å from the plane of the xanthone ring at x, y, z.

Table 1. *Fractional positional parameters* ($\times 10^4$) *of the non-H atoms with e.s.d.'s and equivalent isotropic thermal parameters*

The arithmetic mean of the principal axes of the thermal ellipsoid (Hamilton, 1959):

$$B_{eq} = \tfrac{4}{3}\sum_i\sum_j B_{ij}\mathbf{a}_i.\mathbf{a}_j.$$

|	x	y	z	$B_{eq}(\text{Å}^2)$
C(1)	10985 (4)	2695 (4)	10556 (4)	3·1
C(2)	11023 (5)	3213 (4)	11320 (4)	3·8
C(3)	10213 (5)	3035 (4)	11572 (4)	3·5
C(4)	9414 (4)	2326 (4)	11120 (3)	3·2
C(5)	7605 (4)	−108 (4)	8802 (3)	3·1
C(6)	7421 (4)	−714 (4)	8051 (3)	2·9
C(7)	8094 (4)	−590 (4)	7608 (3)	2·8
C(8)	8928 (4)	108 (4)	7977 (3)	2·6
C(9)	9172 (4)	707 (4)	8777 (3)	2·3
C(10)	8464 (4)	575 (4)	9157 (3)	2·4
C(11)	9391 (4)	1795 (4)	10373 (3)	2·6
C(12)	10159 (4)	1968 (4)	10049 (3)	2·5
C(13)	10076 (4)	1431 (4)	9227 (3)	2·4
C(14)	6999 (5)	−1080 (6)	6063 (4)	5·5
C(15)	9168 (5)	691 (6)	6701 (4)	4·8
O(1)	8581 (3)	1101 (3)	9938 (2)	3·0
O(2)	10747 (3)	1620 (3)	8945 (2)	3·3
O(3)	11758 (3)	2900 (3)	10305 (3)	4·1
O(4)	6624 (3)	−1426 (3)	7695 (2)	3·6
O(5)	7967 (3)	−1226 (3)	6881 (2)	3·3
O(6)	9609 (2)	207 (3)	7572 (2)	2·9
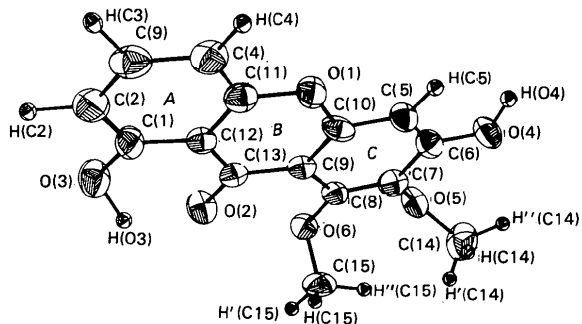
Fig. 1. *ORTEP* plot (Johnson, 1965) of the molecule with 50% probability ellipsoids.
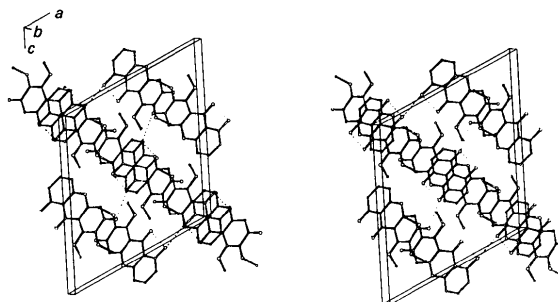

Fig. 2. Stereo packing diagram of the molecules.

The molecules in the crystal are stabilized by intra- and intermolecular hydrogen bonds, $O(3)-H(O3)\cdots O(2)$, $2\cdot582$ (5) Å; $O(3)-H(O3)\cdots O(3)$ ($-x+2\cdot5$, y, $-z+2$), $2\cdot686$ (7) and $O(2)-H(O4)\cdots O(4)$ ($x+0\cdot5$, $-y$, z), $2\cdot825$ Å.

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Structure of N-(2-Amino-6-purinyl)pyridinium Chloride Dihydrate

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Abstract. $C_{10}H_9N_6^+.Cl^-.2H_2O$, $M_r = 284\cdot7$, monoclinic, $P2_1/c$, $a = 7\cdot3671$ (5), $b = 20\cdot938$ (2), $c = 9\cdot219$ (2) Å, $\beta = 116\cdot09$ (1)°, $V = 1277\cdot1$ (3) Å^3, $Z = 4$, $D_x = 1\cdot481$ Mg m^{-3}, $\lambda(Cu K\alpha) = 1\cdot54178$ Å, $\mu = 2\cdot62$ mm^{-1}, $F(000) = 592$, $T = 289$ K, $R = 0\cdot045$ for 1485 observed reflexions. The dimensions of the pyrimidine ring are different from those in other purines; the $N(1)-C(6)-C(5)$ angle is very wide [$121\cdot9$ (2)°]. There is no conjugation between the pyrimidine and pyridinium rings [$C(6)-N^+$(pyridinium) $1\cdot454$ (3) Å]. The three rings composing the cation are coplanar. An intramolecular $C-H\cdots N$ hydrogen bond [$2\cdot974$ (5) Å] cooperates in determining coplanarity between the pyridinium and purine systems. Intermolecular H bonds are arranged in two-dimensional layers perpendicular to a with a single $C-H\cdots O$ link between the layers. The main acceptor center is Cl^- (fivefold) and the donors are the NH and OH (water) groups.

Introduction. We recently reported on the formation (Adamiak, Biała & Skalski, 1985*b*; Adamiak, Biała, Gdaniec, Mielewczyk & Skalski, 1986*a,b*) and reactivity (Skalski, Adamiak & Paszyc, 1984; Adamiak, Biała & Skalski, 1985*a,b*; Adamiak, Biała, Gdaniec, Mielewczyk & Skalski, 1986*a,b*) of nucleobase-derived pyridinium salts as new fluorescent ionic side-products in oligonucleotide synthesis by the phosphotriester method and as synthetic intermediates in nucleoside chemistry. Among various salts of hypoxanthine, guanine, uracil and thymine bases and their ribosides only one, namely N-(2-amino-6-purinyl)pyridinium chloride, has, up to the present, formed crystals of sufficient stability. The title compound was prepared by