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# Conformation of the $O^6$-Alkyl Group in Nucleosides: Structure of 4-Methoxy-1-(β-D-ribofuranosyl)pyrazolo[3,4-*d*]pyrimidine, $C_{11}H_{14}N_4O_5$

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**Abstract.** $M_r = 282{\cdot}3$, monoclinic, $P2_1$, $a = 13{\cdot}015$ (2), $b = 7{\cdot}741$ (1), $c = 6{\cdot}791$ (1) Å, $\beta = 112{\cdot}59$ (1)°, $V = 631{\cdot}7$ (3) Å$^3$, $Z = 2$, $D_m = 1{\cdot}48$, $D_x = 1{\cdot}484$ g cm$^{-3}$, Cu $K\alpha$, $\lambda = 1{\cdot}5418$ Å, $\mu = 10{\cdot}3$ cm$^{-1}$, $T = 294$ K, $F(000) = 296$; the final $R = 0{\cdot}028$ for 1288 reflections ($\geq 2\sigma$). The molecule has the *anti* conformation ($\chi = 71{\cdot}6°$). The ribose has the C(3′)*endo*–C(2′)*exo* ($^3T_2$) pucker with the following pseudorotation parameters: $P = 6{\cdot}3$ (2)° and $\tau_m = 38{\cdot}2$ (2)°. The conformation across C(4′)–C(5′) is *trans*, instead of the preferred $g^+$. The orientation of the $O^6$-alkyl group is 'distal' to the five-membered ring and in spite of the partial shielding of N(1) by the alkyl group, N(1) receives a hydrogen bond from the hydroxyl oxygen O(5′). There is no stacking of the bases in the crystal structure. Molecules related by twofold screw axes are connected to each other by an O(5′)–H(O5′)···N(1) hydrogen bond and form an infinite chain. Molecules related by the **c** translation are on top of each other at 6·6 Å and are linked by an O(2′)–H(O2′)···O(5′) hydrogen bond. An interesting C–H···O hydrogen bond to the ring oxygen O(1′) from C(7)–H is present in the crystal structure.

**Introduction.** Pyrazolo[3,4-*d*]pyrimidine is an analog of purine in which the atoms N(7) and C(8) are interchanged with respect to the purine. Antibiotics such as tubercidin can be viewed as 4-amino-6-aza nucleosides of the above ring system (Suhadolnik, 1970). Several 4-aminopyrazolo[3,4-*d*]pyrimidine derivatives have shown growth-inhibitory activities in tumor cell lines (Hong, De, Tritsch & Chheda, 1976; Sutcliffe, Zee-cheng, Cheng & Robins, 1962) as well as in other biological systems (Krenitsky, Elion, Strelitz & Hitchings, 1967). The pyrazolo[3,4-*d*]pyrimidine ring has provided a very important drug, commonly known as allopurinol, which serves as an excellent inhibitor of xanthine oxidase in man and thereby effectively relieves hyperuricemia condition in gout as well as in certain cancers. It also protects and potentiates the antitumor activity of drugs such as 6-mercaptopurine by preventing the oxidation of the latter by xanthine oxidase to 6-thiouric acid (Rundles & Wyngaarden, 1969; Rundles, 1966).

Of the several nucleosides prepared in our laboratory, the title compound (I) (4-*O*-methylallopurinol riboside) was the most potent against L-1210 mouse leukemia cells *in vitro* ($I_{50}$, $10^{-5}$ *M*). In view of the antitumor activity and also because it is a 4-*O*-methylallopurinol riboside we have carried out a detailed X-ray crystallographic analysis of its molecular structure and conformation (Srikrishnan, Parthasarathy, De & Chheda, 1978). This compound can be regarded as a purine derivative, 6-*O*-methyl-7-aza-8-deazainosine. As a result, the atom numbering in the molecules for the crystallographic work follows that of purine and is different from that for the pyrazolopyrimidine ring system and is given in Fig. 1. For ease of comparison of the X-ray results with other similar compounds, the numbering is similar to those followed in other purine nucleosides; however the standard chemical nomenclature is used elsewhere in the paper.

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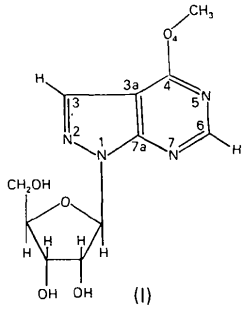


(I)

**Experimental.** Source: 4-chloropyrazolo[3,4-*d*]-pyrimidine was converted into a chloromercury derivative using standard procedures (Davoll & Lowy, 1951; Chheda & Hong, 1971); this derivative was condensed with 2,3,5-tri-*O*-benzoyl-D-ribofuranosyl chloride using a modified coupling procedure (to be published) to give 4-chloro-1-(2′,3′,5′-tri-*O*-benzoyl-β-D-ribofuranosyl)pyrazolo[3,4-*d*]pyrimidine; this was deblocked using 1 *N* NaOMe in methanol at room temperature to yield the title compound. Crystals obtained by slow evaporation from a solution of 1:1 methanol/water mixture; thin transparent needles along **b**; $D_m$ measured by flotation (bromoform/benzene); preliminary X-ray analysis using data from a GE XRD-6 diffractometer and final refinements using data from a CAD-4 diffractometer; accurate unit-cell parameters on a CAD-4 diffractometer using 25 reflections with $\theta > 25°$; a thin crystal of dimensions $0{\cdot}3 \times 0{\cdot}2 \times 0{\cdot}15$ mm used for three-dimensional data (to the limit of $2\theta = 150°$ for Cu $K\alpha$ radiation) by the $\omega/2\theta$ scan; scan widths calculated using the expression $(0{\cdot}5 + 0{\cdot}15 \tan\theta)°$, and aperture widths using $(3{\cdot}0 + 1{\cdot}2 \tan\theta)$ mm; maximum time spent on any reflection measurement 100 s; a faster scan was used for strong reflections; intensities of three reflections monitored after every hour of exposure: variation in intensity <3% during the complete data collection; orientation matrix checked every 100 reflections; 1459 reflections measured, out of which 1288 significant ($\geq 2\sigma$); Lorentz and polarization corrections applied; intensities of three reflections at $\chi \sim 90°$ measured for all values of $\varphi$ from 0 to 360° and the resultant curve of transmission as a function of $\varphi$ used to calculate the absorption for all the reflections: average transmission factor 0·84; structure solved using *MULTAN* (Germain, Main & Woolfson, 1971) and trial-and-error method; 255 $E$ values ($|E| > 1{\cdot}3$) used as input to *MULTAN* and the correct set with the highest figure of merit of 1·049 and a residual value of 0·36 gave the pyrazolopyrimidine ring but not the ribose; remaining atoms found from successive electron density maps after least-squares refinement of nine atoms of the base; refinements with individual anisotropic thermal parameters led to $R$ 0·061; $\Delta\rho$ map computed at this stage revealed the positions of all the H atoms in the structure; final cycles of refinement with anisotropic thermal parameters for the non-hydrogen atoms led to $R$ 0·028 for the 1288 observed reflections; $\sum w[|F_o|^2 - (1/K)|F_c|^2]^2$ minimized, where $w = 1/\sigma^2(|F_o|^2)$ and $K$ is the scale factor. Programs and atomic scattering factors as in the CAD-4 structure determination package; Fourier and torsion-angle programs by Dr S. T. Rao and *ORTEP* by Johnson (1965).

**Discussion.** The final positional parameters for the non-hydrogen atoms and for the H atoms are given in Table 1.* The bond distances and bond angles are given in Figs. 1(*a*) and 1(*b*) respectively. Bond angles involving the H atoms are in the usual range for X-ray determination.

The bond distances and angles in the pyrazolo-[3,4-*d*]pyrimidine base may be compared to those found in 8-azatubercidin (Sprang, Scheller, Rohrer & Sundaralingam, 1978), allopurinol (Prusiner & Sundaralingam, 1972) and 5*H*-pyrazolo[3,4-*d*]pyrimidine-4-thione (Gadret, Goursolle & Leger, 1974), remembering, however, that the double-bond character of

* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplenentary Publication No. SUP 38684 (9 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. *Final positonal parameters, equivalent isotropic thermal parameters for the non-hydrogen atoms, and isotropic thermal parameters for hydrogen atoms, with estimated standard deviations in parentheses*

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

| | $x$ | $y$ | $z$ | $B_{eq}$ or $B$(Å$^2$) |
|---|---|---|---|---|
| O(6) | 1·0663 (1) | 0·0903 (3) | 0·5031 (2) | 4·33 (6) |
| O(1′) | 0·7203 (1) | 0·0651 (2) | 0·9633 (2) | 2·91 (4) |
| O(2′) | 0·5836 (1) | 0·3850 | 0·9221 (3) | 4·42 (5) |
| O(3′) | 0·4318 (1) | 0·1639 (3) | 0·6497 (2) | 3·63 (5) |
| O(5′) | 0·6445 (1) | −0·2768 (2) | 1·0073 (2) | 3·43 (4) |
| N(1) | 1·1173 (1) | 0·2219 (3) | 0·8325 (3) | 3·64 (6) |
| N(3) | 0·9812 (2) | 0·2905 (3) | 0·9804 (3) | 3·66 (5) |
| N(8) | 0·7441 (1) | 0·1314 (4) | 0·5486 (3) | 3·77 (6) |
| N(9) | 0·7943 (1) | 0·2068 (3) | 0·7449 (2) | 3·15 (5) |
| C(2) | 1·0822 (2) | 0·2874 (4) | 0·9821 (3) | 3·93 (7) |
| C(4) | 0·9062 (2) | 0·2218 (3) | 0·7990 (3) | 2·85 (6) |
| C(5) | 0·9282 (2) | 0·1540 (4) | 0·6314 (3) | 3·09 (6) |
| C(6) | 1·0404 (2) | 0·1564 (3) | 0·6577 (3) | 3·28 (6) |
| C(*M*6) | 1·1807 (2) | 0·0949 (5) | 0·5262 (4) | 4·59 (8) |
| C(7) | 0·8237 (2) | 0·0999 (4) | 0·4794 (3) | 3·79 (8) |
| C(1′) | 0·7447 (2) | 0·2291 (4) | 0·8826 (3) | 2·85 (6) |
| C(2′) | 0·6179 (2) | 0·3046 (3) | 0·7713 (3) | 3·33 (6) |
| C(3′) | 0·5462 (2) | 0·1420 (3) | 0·6987 (3) | 2·87 (6) |
| C(4′) | 0·6040 (2) | 0·0203 (3) | 0·8868 (3) | 2·60 (5) |
| C(5′) | 0·5904 (2) | −0·1665 (3) | 0·8264 (3) | 3·15 (6) |
| H(C2) | 1·141 (2) | 0·334 (6) | 1·110 (4) | 5·2 (8) |
| H(C7) | 0·803 (3) | 0·053 (6) | 0·337 (5) | 5·7 (8) |
| H*a*(C*M*6) | 1·228 (3) | 0·020 (6) | 0·652 (5) | 5·5 (8) |
| H*b*(C*M*6) | 1·186 (3) | 0·048 (6) | 0·400 (5) | 6·5 (9) |
| H*c*(C*M*6) | 1·209 (2) | 0·213 (5) | 0·544 (4) | 4·8 (7) |
| H(C1′) | 0·780 (2) | 0·300 (5) | 0·996 (4) | 4·3 (6) |
| H(C2′) | 0·614 (2) | 0·389 (5) | 0·654 (4) | 4·6 (7) |
| H(O2′) | 0·609 (2) | 0·487 (6) | 0·949 (5) | 5·5 (8) |
| H(C3′) | 0·554 (2) | 0·097 (4) | 0·566 (3) | 2·6 (4) |
| H(O3′) | 0·425 (2) | 0·219 (5) | 0·768 (5) | 4·9 (7) |
| H(C4′) | 0·575 (2) | 0·053 (4) | 1·006 (4) | 3·0 (5) |
| H*a*(C5′) | 0·617 (2) | −0·187 (4) | 0·717 (4) | 3·3 (5) |
| H*b*(C5′) | 0·511 (3) | −0·194 (5) | 0·772 (5) | 5·0 (7) |
| H(O5′) | 0·722 (2) | −0·264 (5) | 1·060 (4) | 5·0 (7) |

C(6)–O(6) changes due to alkylation. The glycosidic bond length of 1·437 (3) Å in this structure is shorter than the corresponding bond length of 1·460 (5) Å in 8-azatubercidin (Sprang *et al.*, 1978). The endocyclic angle at N(8) is smaller by 4–6° than the corresponding value at C(8)–H in purine systems, as had been observed in formycin monohydrate (Prusiner, Brennan & Sundaralingam, 1973). This decrease is accompanied by a concomitant increase of the angles at N(9) and C(7) and a decrease of the angle C(4)–C(5)–C(7) similar to that found in 8-azatubercidin, allopurinol and 5*H*-pyrazolo[3,4-*d*]pyrimidine-4-thione.

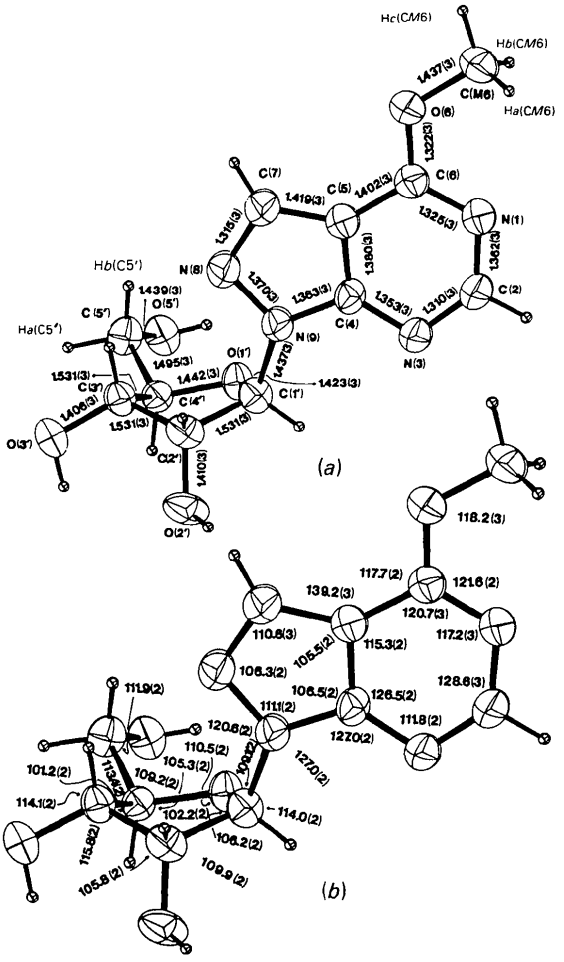


Fig. 1. (*a*) Bond distances (Å). Note that the conformation of the $O^6$-methyl group is distal to the five-membered ring. (*b*) Bond angles (°) in the molecule. The e.s.d.'s given in parentheses refer to the last digit. The molecule has the *anti* conformation ($\chi = 71{\cdot}6°$). The ribose has the C(3′)*endo*–C(2′)*exo* ($^3T_2$) pucker and the conformation across C(4′)–C(5′) is *trans* instead of the preferred $g^+$. [C(2)–H(C2) 0·98 (3), C(7)–H(C7) 0·97 (4), C(*M*6)–H*a*(C*M*6) 1·02 (4), C(*M*6)–H*b*(C*M*6) 0·96 (4), C(*M*6)–H*c*(C*M*6) 0·97 (4), C(1′)–H(C1′) 0·94 (3), C(2′)–H(C2′) 1·02 (3), O(2′)–H(O2′) 0·85 (4), C(3′)–H(C3′) 1·01 (2), O(3′)–H(O3′) 0·94 (3), C(4′)–H(C4′) 1·05 (3), C(5′)–H*a*(C5′) 0·94 (3), C(5′)–H*b*(C5′) 0·98 (4), O(5′)–H(O5′) 0·94 (3) Å.]

Table 2. *Some selected torsion angles* (°), *with estimated standard deviations in parentheses*

| | | | |
|---|---|---|---|
| N(8)–N(9)–C(1′)–O(1′) | 71·6 (3) | O(1′)–C(1′)–C(2′)–C(3′) | −28·8 (3) |
| C(1′)–C(2′)–C(3′)–C(4′) | 37·2 (3) | C(3′)–C(4′)–C(5′)–O(5′) | −179·3 (3) |
| C(2′)–C(3′)–C(4′)–O(1′) | −33·4 (4) | O(1′)–C(4′)–C(5′)–O(5′) | 63·7 (3) |
| C(3′)–C(4′)–O(1′)–C(1′) | 16·3 (3) | N(1)–C(6)–O(6)–C(*M*6) | −1·6 (4) |
| C(4′)–O(1′)–C(1′)–C(2′) | 8·1 (3) | C(5)–C(6)–O(6)–C(*M*6) | 178·8 (3) |

The conformation about the glycosyl bond ($\chi = 71{\cdot}6°$) is at the high end of the *anti* range. The exocyclic angles around N(9) are sensitive to the glycosyl torsion angle (Sprang *et al.*, 1978). In cases where it is *anti*, the C(4)–N(9)–C(1′) angle is smaller than C(8)–N(9)–C(1′) by about 2 to 6° and this trend is reversed for *syn* nucleosides. In our case the N(8)–N(9)–C(1′) angle is smaller than the C(4)–N(9)–C(1′) angle by 6·4°, though the conformation is *anti*.

The least-squares plane through the nine atoms of the base ring is given by the equation $-0{\cdot}033X - 0{\cdot}900Y + 0{\cdot}434Z = 4{\cdot}895$ where $X$, $Y$ and $Z$ are the atomic coordinates in Å referred to the crystallographic $a, b$ and $c^*$ axes. All the atoms of the base are within 0·007 Å of this plane but O(6) and C(1′) are displaced on the same side of this plane by 0·022 and 0·262 Å respectively. The dihedral angle between the pyrimidine and the pyrazolo rings is 0·5° and is similar to the values found in purine and its analogs.

The ribose assumes a C(3′)*endo*–C(2′)*exo* ($^3T_2$) pucker with C(3′) and C(2′) deviating from the mean plane of the other three atoms by 0·41 and −0·21 Å respectively. In terms of the pseudorotation model (Altona & Sundaralingam, 1972) the ribofuranosyl ring has a pseudorotation angle $P$ of 6·3 (2)° and a maximum amplitude of pucker $\tau_m = 38{\cdot}2$ (2)°. Some of the selected conformational parameters are given in Table 2.

The most interesting conformational features of the molecule are the distal conformation of the $O^6$-alkyl group and the *trans* conformation across the C(4′)–C(5′) bond. The torsional angles C(3′)–C(4′)–C(5′)–O(5′) and O(1′)–C(4′)–C(5′)–O(5′) are −179·3 (3) and 63·7 (3)° respectively. A similar *trans* conformation has also been found in the structure of 8-azatubercidin and 6-azauridine 5′-monophosphate (Saenger & Suck, 1973). The high-*anti* conformation along with the non-standard conformation *trans* or *gauche*$^-$ across the C(4′)–C(5′) bond, leading to proper positioning of O(5′) and another keto oxygen, has been suggested to be associated with the blocking of the enzymatic activity of orotidylic acid decarboxylase by 6-azauridine 5′-monophosphate (Saenger, Suck, Knappenberg & Dirkx, 1979). It is interesting to note that the conformation of the title compound has similar conformational features, but further work is necessary before one can discuss the activity of the title compound against L-1210 mouse cells in any great detail.

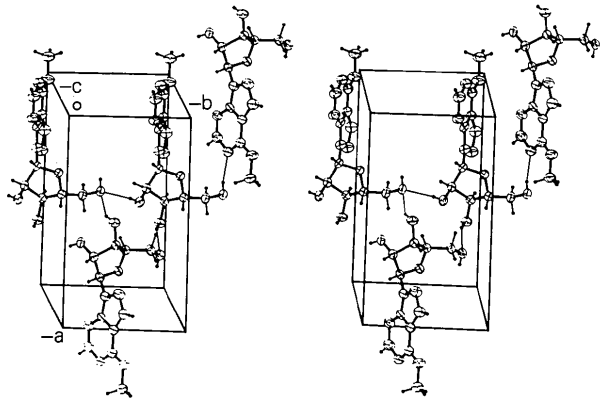


Fig. 2. A stereoscopic view of the hydrogen bonding and packing of the molecules in the crystal structure. Molecules related by a twofold screw axis are connected to each other by an O(5′)–H(O5′)···N(1) hydrogen bond [O(5′)···N(1), 2·864 (2); H(O5′)···N(1), 1·94 (5) Å, O(5′)–H(O5′)···N(1), 171°]. Molecules related by **c** translation are on top of each other at 6·6 Å and linked by an O(2′)–H(O2′)···O(5′) hydrogen bond [O(2′)···O(5′), 2·733 (1); H(O2′)···O(5′), 2·07 (5) Å, O(2′)–H(O2′)···O(5′), 172°].

The molecules are linked by O(5′)–H(O5′)···N(1) hydrogen bonding (Fig. 2). The methoxy group is distal to the ribose and partially shields N(1) from hydrogen bonding; the shortest contacts of O(5′) with two of the three methyl H atoms are 2·49 and 2·46 Å. Other orientations of the methyl group across O(6)–C(*M*6) will introduce shorter H···O(5′) contacts. In addition to the hydrogen bond from O(2′) shown in Fig. 2, O(5′) is also the acceptor of a hydrogen bond from O(3′) [O(3′)···O(5′), 2·899 (1); H(O3′)···O(5′), 2·05 (3) Å; O(3′)–H(O3′)···O(5′), 149°]. There is a C–H···O hydrogen bond in the structure involving the furanose ring oxygen O(1′) as an acceptor [C(7)···O(1′), 3·248 (2); H(C7)···O(1′), 2·35 (4) Å; C(7)–H(C7)···O(1′), 154°]. The acceptance of a hydrogen bond by O(1′) is rather unusual in normal nucleosides and nucleotides but not uncommon in modified nucleosides (Sprang & Sundaralingam, 1973; Srikrishnan, Fridey & Parthasarathy, 1979; Taylor & Kennard, 1982).

The packing of the molecules in the crystal structure is shown in Fig. 2. There is hardly any stacking of the bases in the crystal structure. This is surprising, since 8-azatubercidin and allopurinol as well as 6-methoxypurine riboside (Cook, Gartland & Bugg, 1980) have good stacking of the bases in their respective crystal structures.

The distal orientation of the methyl group in the structure indicates that such a conformational preference is also possible for $O^6$-alkylguanines (Srikrishnan *et al.*, 1978; Cook *et al.*, 1980). Since the attack on the $O^6$-position of guanine by alkylating agents and chemical carcinogens (Loveless, 1969) is particularly significant, it is important to examine the effect of such base modifications on nucleic acids (Mehta & Ludlum, 1976). The presence of $O^6$-methylguanine in a template leads to misincorporation (Gerchman, Dombrowski & Ludlum, 1972); also poly($O^6$-methyl-GMP) does not form helices with poly(U). Due to alkylation, N(1) of guanine will become a hydrogen-bond acceptor instead of a donor and hence cannot base-pair with C. If the orientation of the $O^6$-alkyl group is proximal, then $O^6$-methylguanine can pair with U, using the N(1) and N(2)H of guanine and the N(3)H and O(2) of uracil. But our results indicate that the distal orientation of the $O^6$-alkyl group will prevent any base-pairing with U, agreeing with the result that poly($O^6$-methyl-GMP) does not form any stable complex with poly(U).

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# Structure of Phenacetin, $C_{10}H_{13}NO_2$*

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**Abstract.** $M_r = 179{\cdot}21$, monoclinic, $P2_1/c$, $a = 13{\cdot}25\ (2)$, $b = 9{\cdot}65\ (1)$, $c = 7{\cdot}81\ (1)$ Å, $\beta = 104{\cdot}9\ (5)°$, $V = 965\ (2)$ Å$^3$, $Z = 4$, $D_m = 1{\cdot}240\ (4)$, $D_x = 1{\cdot}234\ (3)$ Mg m$^{-3}$, Cu $K\alpha$, $\lambda = 1{\cdot}5418$ Å, $\mu = 0{\cdot}66$ mm$^{-1}$, $F(000) = 384$, $T = 300$ K, $R = 0{\cdot}088$ for 1459 observed reflections. The planes of the side groups O(7)C(8)C(9) and N(10)C(11)C(12)O(13) are tilted with respect to the plane of the benzene ring by 9 (1) and 29 (1)°, respectively. The nitrogen and oxygen atoms of the acetamido group from two symmetry-related molecules are hydrogen bonded. The crystal structure is stabilized by hydrogen bonds and van der Waals forces.

**Introduction.** Phenacetin is the most prominent pain-relieving drug among acetanilide derivatives. We determined the structure of phenacetin as a part of our programme of structure analysis of drugs (Tiwari, Patel & Singh, 1982). A preliminary account of the structure has already been made (Patel, Patel & Singh, 1982) and the structure refinement and discussion are reported here.

**Experimental.** Hexagonal plate-shaped crystals from solution in methanol at 277 K; unit-cell parameters from 34 reflections on oscillation and Weissenberg photographs, systematic absences indicated $P2_1/c$, $D_m$ by flotation in a mixture of benzene and carbon tetrachloride; crystals elongated along [001]; crystal $0{\cdot}33 \times 0{\cdot}10 \times 0{\cdot}09$ mm, multiple films, equi-inclination Weissenberg technique, Ni-filtered Cu radiation; 1459 independent reflections, reciprocal levels $hkL$, $L = 0$–7, $2\theta_{max} = 154°$, 455 unobserved reflections $I < 3\sigma(I)$; intensities estimated visually with calibrated film strips, corrected for Lorentz and polarization effects and spot-shape distortions but not for absorption ($\mu r = 0{\cdot}07$); programs used in the above calculations were written by the authors.

The positions of 10 out of 13 non-hydrogen atoms in the asymmetric unit obtained with *MULTAN* (Germain, Main & Woolfson, 1971), Fourier methods revealed remaining three atoms; subsequent isotropic and anisotropic refinement cycles, on $F$, of non-hydrogen atoms by block-diagonal least squares [program originally written by Shiono (1968–1971) and modified by the authors], $R = 0{\cdot}098$; all hydrogen atoms located from difference Fourier, positional and isotropic thermal parameters of hydrogen refined, $R = 0{\cdot}088$ for 1459 observed reflections; in final cycles, $\Delta_{av}$ and $\Delta_{max}$ for non-hydrogen and hydrogen atoms were $0{\cdot}04\sigma$ and $0{\cdot}12\sigma$, and $0{\cdot}11\sigma$ and $0{\cdot}3\sigma$, respectively; $w = 1/(a + bF_{obs} + cF_{obs}^2)$ (Cruickshank, 1961), adjusted to make the average $w\Delta^2$ independent of $F_{obs}$, $a = 1{\cdot}0$, $b = 0{\cdot}05$ and $c = 0{\cdot}001$, $R_w = 0{\cdot}091$; atomic scattering factors from Cromer & Waber (1965) for non-H atoms, and from Stewart, Davidson & Simpson (1965) for H atoms; $\Delta\rho$ excursions $<0{\cdot}13$ e Å$^{-3}$.† All calculations were performed on the IBM 360/44 computer system of the M. S. University of Baroda, Baroda.

**Discussion.** Final positional and equivalent isotropic thermal parameters are listed in Table 1.

Fig. 1 shows a stereoscopic illustration and the numbering scheme of the molecule (*ORTEP*: Johnson, 1965). Bond distances and angles of non-hydrogen atoms and relevant torsion angles are given in Table 2. The O(7) atom deviates from the plane of the benzene ring by 0·01 (2) Å, whereas N(10) is displaced by 0·04 (2) Å. The planes of the $C_2H_5O$ moiety and that of the acetamido group are inclined with respect to the

* *p*-Ethoxyacetanilide.

† Lists of structure factors, anisotropic thermal parameters, H-atom parameters, bond lengths and angles involving H and least-squares-planes' data have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 38687 (11 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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