

cell. Fig. 2 shows the packing of the unit cell projected on the *ac* plane.

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Structure of 2-Amino-4-methylphenol

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Abstract. C₇H₉NO, *M_r* = 123.15, orthorhombic, *Pbca*, *a* = 7.7803 (7), *b* = 22.901 (2), *c* = 7.5962 (6) Å, *V* = 1353.5 (2) Å³, *Z* = 8, *D_m* = 1.20, *D_x* = 1.206 Mg m⁻³, λ(Cu *Kα*) = 1.5418 Å, μ = 0.62 mm⁻¹, m.p. 410–413 K, *F*(000) = 528, *T* = 293 K, final *R* = 0.061 for 999 non-zero reflections. The molecules are held together by N–H...O and O–H...N hydrogen bonds to form a sheet parallel to (010). The sheets are stacked along *b* by weak van der Waals interactions. The *sp*³ character of the amino group is evidenced by the C–N length, 1.417 (3) Å, the N-atom deviation from the benzene ring plane, 0.110 (3) Å, and the sum of the angles about N, 333 (1)°. The crystal and molecular structures are comparable with those of 2-aminophenol.

Introduction. Morphotropism in the crystal structures of the derivatives of 2-aminophenol is of particular interest, because the structure of 2-aminophenol shows remarkable correspondence to that of benzene (*Pbca*) (Haisa, Kashino & Kawashima, 1980). Among the derivatives of 2-aminophenol, the structure of 2-amino-4-chlorophenol (*P2₁/c*, maximal subgroup of *Pbca*) has already been determined (Ashfaquzzaman & Pant, 1979). In the present work the structure of 2-amino-4-methylphenol has been determined in order to obtain

information on the effect of the 4-methyl group, which is similar in size to the 4-Cl atom, on the crystal structure of 2-aminophenol (Ashfaquzzaman & Pant, 1979).

Experimental. Crystals grown by slow evaporation from ethanol, brown plates with developed faces {010}. *D_m* by flotation in aqueous KI. Systematic absences *0k1* for *k* odd, *h0l* for *l* odd, *hk0* for *h* odd, space group *Pbca*. Crystal 0.24 × 0.12 × 0.20 mm. Rigaku AFC-5 four-circle diffractometer. Lattice parameters determined with 20 reflections in the range 15 < 2θ < 48° by least-squares method; intensities measured up to (sinθ)/λ 0.5753 Å⁻¹, ω–2θ scan method [scan speed 4° min⁻¹ in ω, scan range (2θ): 1.2° + 0.15° tanθ], Ni-filtered Cu *Kα*, 40 kV, 200 mA (rotating anode), background measured for 4 s on either side of the peak. Three standard reflections measured for every 57 reflections, fluctuation within 2.2% in *F*. Lorentz and polarization corrections; no absorption correction. All 1076 unique reflections (ranging over *h* = 0 to 8, *k* = 0 to 26, *l* = 0 to 8) used for refinement; 936 reflections with *F_o* > 1.0σ(*F_o*). Structure solved by Patterson method, and refined (anisotropically for non-H atoms) by block-diagonal least squares; ∑w(|*F_o*| – |*F_c*|)² minimized, with *w* = 1.0/(σ(*F_o*))² – 0.0552|*F_o*| +

$0.0029 |F_o|^2$ for $|F_o| > 0$, $w = 0.8267$ for $|F_o| = 0$; H-atom positions determined from difference Fourier map, and refined isotropically by least squares. Extinction correction for 17 strongest reflections [$I_{\text{corr}} = I_o(1 + 4.89 \times 10^{-5} I_o)$]. $R = 0.061$ for 999 non-zero reflections, $wR = 0.053$, $S = 1.32$, $(\Delta/\sigma)_{\text{max}}$ in final refinement cycle 0.4; max. and min. $\Delta\rho$ in final difference Fourier map 0.22 and $-0.17 \text{ e } \text{\AA}^{-3}$, atomic scattering factors from *International Tables for X-ray Crystallography* (1974), computations carried out at the Crystallographic Research Center, Institute for Protein Research, Osaka University, and at the Okayama University Computer Center; programs *HBL5-V* and *DAPH* (Ashida, 1973), *MOLCON* (Fujii, 1979), and *ORTEP* (Johnson, 1965).

Table 1. Final atomic coordinates ($\times 10^4$) and equivalent isotropic thermal parameters with e.s.d.'s in parentheses

$$B_{\text{eq}} = \frac{4}{3} \sum \beta_{ii} / a_i^2.$$

	x	y	z	$B_{\text{eq}}(\text{\AA}^2)$
O	2343 (2)	38.2 (5)	700 (2)	3.45 (6)
N	850 (2)	649.6 (6)	-1913 (2)	3.09 (6)
C(1)	2918 (2)	597.5 (7)	463 (2)	2.69 (7)
C(2)	2102 (2)	924.5 (7)	-841 (2)	2.49 (7)
C(3)	2616 (2)	1494.9 (7)	-1131 (2)	2.90 (8)
C(4)	3943 (2)	1751.6 (7)	-165 (2)	3.14 (8)
C(5)	4739 (3)	1416.2 (8)	1110 (3)	3.62 (9)
C(6)	4239 (3)	844.4 (8)	1430 (3)	3.41 (8)
C(7)	4455 (3)	2376.9 (8)	-498 (3)	4.5 (1)

Table 2. Bond lengths (\AA) and interbond angles ($^\circ$) with e.s.d.'s in parentheses

O—C(1)	1.369 (2)	C(3)—C(4)	1.396 (3)
N—C(2)	1.417 (3)	C(4)—C(5)	1.383 (3)
C(1)—C(2)	1.395 (3)	C(4)—C(7)	1.508 (4)
C(1)—C(6)	1.384 (3)	C(5)—C(6)	1.387 (3)
C(2)—C(3)	1.384 (3)		
O—C(1)—C(2)	116.6 (2)	C(2)—C(3)—C(4)	121.8 (2)
O—C(1)—C(6)	123.7 (2)	C(3)—C(4)—C(5)	117.7 (2)
C(2)—C(1)—C(6)	119.7 (2)	C(3)—C(4)—C(7)	120.5 (2)
N—C(2)—C(1)	118.8 (2)	C(5)—C(4)—C(7)	121.8 (2)
N—C(2)—C(3)	121.8 (2)	C(4)—C(5)—C(6)	121.4 (2)
C(1)—C(2)—C(3)	119.2 (2)	C(1)—C(6)—C(5)	120.1 (2)

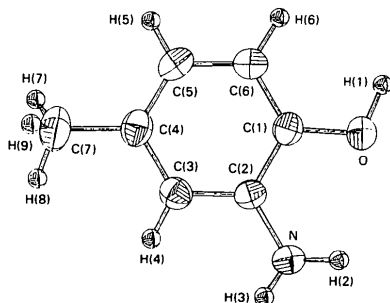


Fig. 1. The thermal ellipsoids of the molecule with atomic numbering. Ellipsoids of 50% probability are drawn for the non-H atoms; the H atoms are represented as spheres equivalent to $B = 1.0 \text{ \AA}^2$.

Discussion. Final atomic parameters are listed in Table 1.* The thermal ellipsoids of the molecules are shown in Fig. 1, with atomic numbering. Bond lengths and interbond angles are listed in Table 2.

The benzene ring is planar within $0.004 (3) \text{ \AA}$. O and C(7) deviate only by $0.010 (3)$ and $0.026 (4) \text{ \AA}$, respectively, from the benzene ring plane, but the deviation of N, $-0.110 (3) \text{ \AA}$, is remarkable as found in 2-aminophenol (Ashfaquzzaman & Pant, 1979). The C(2)—N length and the sum of the angles about N, $333(1)^\circ$, correspond to values at the pyramidal N atom in anilines (Stålhandske, 1976), but the C—N length is shorter than the typical $C(sp^3)$ —N length of 1.47 \AA found in 2-aminophenol hydrochloride (Cesur & Richards, 1965). The linear relationship between the degree of pucker at the amino N and the C—N lengths (Chao & Schempp, 1977) holds there. The inner angle at C(4) is smaller than the sp^2 angle as found in many methyl-substituted benzene derivatives (Domenicano, Vacigo & Coulson, 1975).

The projection of the crystal structure viewed along **a** is shown in Fig. 2. The molecules related by 2_1 along **c** are held together by O—H...N hydrogen bonds [O...Nⁱⁱⁱ $2.783 (2)$, O—H(1) $0.99 (2)$, H(1)...Nⁱⁱⁱ $1.81 (2) \text{ \AA}$, O—H(1)...Nⁱⁱⁱ $171 (2)$, H(1)...Nⁱⁱⁱ—C(2ⁱⁱⁱ) $108.1 (7)^\circ$]. In addition, the molecules related by $\bar{1}$ are held together by O...H—N hydrogen bonds [O...Nⁱⁱ $3.082 (2)$, O...H(2ⁱⁱ) $2.22 (2)$, H(2ⁱⁱ)—Nⁱⁱ $0.97 (2) \text{ \AA}$, O...H(2ⁱⁱ)—Nⁱⁱ $148 (2)^\circ$]. A sheet parallel to (010) is formed by these two kinds of hydrogen bonds. In the sheet the benzene rings related by an *a* glide plane are arranged with a dihedral angle δ of $85.01 (7)^\circ$ as in

* Lists of structure factors, anisotropic thermal parameters, H-atom parameters and bond lengths and angles involving H atoms have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44626 (9 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

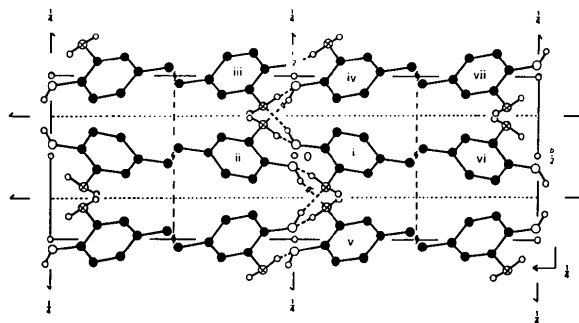


Fig. 2. Projection of the crystal structure viewed along **a** (○:O, ⊙:N, ●:C, ○:H). The H atoms attached to the C atoms are omitted. Hydrogen bonds are shown by broken lines. Symmetry code: (i) x, y, z ; (ii) $-x, -y, -z$; (iii) $\frac{1}{2}-x, -y, \frac{1}{2}+z$; (iv) $\frac{1}{2}+x, y, \frac{1}{2}-z$; (v) $\frac{1}{2}+x, y, -\frac{1}{2}-z$; (vi) $\frac{1}{2}+x, \frac{1}{2}-y, -z$; (vii) $x, \frac{1}{2}-y, \frac{1}{2}+z$.

benzene ($\delta = 85.0^\circ$) (Cox, Cruickshank & Smith, 1958) and 2-aminophenol ($\delta = 87.7^\circ$) (Ashfaqzaman & Pant, 1979; Haisa *et al.*, 1980). The second H of the amino group is free from any hydrogen bond, the shortest contact involving the H being 2.66 (2) Å for C(3)···H(3^v). The sheets are stacked along **b** by weak van der Waals interactions in accordance with the morphology of the crystals.

The modes of hydrogen bonding, the sheet formation and the sheet stacking are the same as those in 2-aminophenol. However, a change in the mode of sheet stacking is found in 2-amino-4-chlorophenol, where the symmetry operation for the sheet stacking is changed from 2₁ along **b** to an a translation. Thus, the space group descends to $P2_1/c$, a maximal subgroup of $Pbca$. Such a descent in space group is found between benzene ($Pbca$ form) and some of its derivatives; e.g. the $P2_1/c$ form of benzene (Mighell, Weir & Block, 1969), naphthalene ($P2_1/a$, Cruickshank, 1957) and biphenyl ($P2_1/a$, Charbonneau & Delugeard, 1977).

In 3- and 4-aminophenols (de Rango, Brunie, Tsoucaris, Declercq & Germain, 1974; Brown, 1951), centrosymmetric pairing of the molecules through hydrogen bonds between the amino and hydroxy groups is prohibited by packing requirements, the only possible mode of hydrogen bonding being the formation of endless chains of the molecules. Thus, the crystals of 3- and 4-aminophenols adopt non-centrosymmetric space groups ($Pca2_1$ and $Pna2_1$, respectively). It should be noted that both of these space groups are also subgroups of $Pbca$.

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Structure of Hypoxanthine

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Abstract. 1,7-Dihydro-6H-purin-6-one, $C_5H_4N_4O$, $M_r = 136.11$, triclinic, $P\bar{1}$, $a = 7.102$ (2), $b = 9.759$ (2), $c = 10.387$ (2) Å, $\alpha = 58.85$ (2), $\beta = 67.64$ (2), $\gamma = 72.00$ (2)°, $V = 564.0$ (2) Å³, $Z = 4$, $D_x = 1.60$, $D_m = 1.60$ g cm⁻³, $\lambda(\text{Mo } K\alpha) = 0.71073$ Å, $\mu = 0.78$ cm⁻¹, $F(000) = 280$, room temperature, $wR = 4.6\%$ for 2916 observed unique reflections. Hypoxanthine exhibits a layered structure of N–H···O and N–H···N hydrogen-bonded molecules, the mean stacking distance between molecules of adjacent layers being

3.25 Å. There are two crystallographically independent molecules in the structure; in both of them the 1H,9H tautomer (lactam configuration) is the predominant form.

Introduction. Hypoxanthine occasionally occurs as a constituent of the nucleoside inosine in minor amounts in transfer RNA (Hurst, 1980), and it is an intermediate product of purine metabolism formed by degradation of nucleic acids. Hypoxanthine is oxidized to xanthine and uric acid in man, these reactions being catalyzed by the molybdenum- and iron-containing

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