C_{za} and C_{xc}, C_{yc} are the coordinates, and T_a and T_c the translation components of the screw axes parallel to **a** and **c**, respectively. By means of the y coordinates of the two independent molecules, the y origin in $P2_1$ was chosen such that the pseudo 2_1 axes parallel to **a** and **c** lie at $y = 0$ and $y = \frac{1}{4}$, respectively, expressed by the calculated values for C_{ya} and C_{yc}, giving 0·001 (1) and 0·250 (5), respectively. The x and z coordinates of the independent molecules were used to calculate the other unknowns, giving $T_a = 0.52$ (6), $C_{za} = 0.25$ (1) and $T_c = 0.50$ (2) and $C_{xc} = 0.26$ (3). Although the pseudo 2_1 axis parallel to **c** is not exactly at $x = \frac{1}{4}$, it has a mean translation of $\frac{1}{2}$**c** and this ought to give rise to very weak $00l$ reflections with $l = 2n + 1$, in accordance with experimental observations. The mean translation for the pseudo 2_1 axis parallel to **a** is significantly different from $\frac{1}{2}$**a**, and consequently no relative weak $h00$ reflections with $h = 2n + 1$ have been observed. Assuming exact $P2_12_12_1$ symmetry results in a mean deviation of atom positions of 0·52 (4) Å for both molecules.

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Structure of 2-(4-Methyl-2-pyridyliminomethyl)phenol, C₁₃H₁₂N₂O
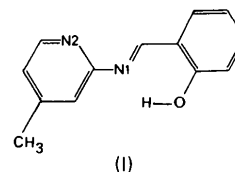
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Abstract. $M_r = 212·0$, monoclinic, $P2_1/c$, $a = 11·772$ (4), $b = 7·5386$ (7), $c = 15·154$ (5) Å, $\beta = 124·89$ (2)° (JCPDS Diffraction File No. 33–1999) [reduced cell: $P2_1/n$, $a' = a$, $b' = b$, $c' = 12·812$ (5) Å, $\beta' = 104·02$ (5)°], $V = 1103·1$ (4) Å³, $Z = 4$, $D_m = 1·24$ (3) (flotation in dioxane and bromoform), $D_x = 1·276$ (1) Mg m⁻³, $\lambda(\text{Mo }K\alpha) = 0·7107$ Å, $\mu = 0·09$ mm⁻¹, $F(000) = 448·0$. The final R is 0·079 for 875 observed reflections. The molecule has an O–H⋯N hydrogen bond contained in the plane of the salicylidene ring. The pyridine ring is twisted by ~12 (1)° from the rest of the molecule. The H atom of the exocyclic C atom is *cis* with respect to the N atom of the pyridine ring.

Introduction. The structure of 2-(4-methyl-2-pyridyliminomethyl)phenol (I) has been determined as a preliminary step in the synthesis and structural study of copper(II) complexes with Schiff bases derived from salicylaldehyde and 2-aminopyridine as ligands.

(I)

Experimental. Dark-yellow crystals (from methanol solution), $0.20 \times 0.08 \times 0.30$ mm, Philips PW 1100 diffractometer, graphite-monochromatized Mo $K\alpha$, $\omega/2\theta$ scan mode, two standard reflections every 55 measurements (variation $\pm 2\%$), 2425 $\pm hkl$ with $2\theta < 54°$, 2343 independent, $R_{int} = 0.043$ from merging 82 equivalent $hk0$ pairs, 1468 unobserved with $I \le 2.5\sigma(I)$, Lp correction, absorption and anomalous dispersion ignored, 41 reflections with $2\theta < 39°$ used for refining cell parameters (the matrix $100/0\overline{1}0/\overline{1}0\overline{1}$ relates the two sets of parameters given in the Abstract); direct methods (*MULTAN*76; Main, Lessinger, Woolfson, Germain & Declercq, 1976), anisotropic full-matrix refinement using F magnitudes, H of OH group from ΔF synthesis refined with fixed isotropic U, other H atoms calculated (bond length 1 Å); final $R = R_w = 0.079$, $w = 1$, $\Delta/\sigma < 0.02$, residual $\Delta\rho \pm 0.25$ e Å^{-3}; scattering factors for O, N, C from Cromer & Mann (1968), for H from Stewart, Davidson & Simpson (1965). Computer programs: XRAY76 system (Stewart, Machin, Dickinson, Ammon, Heck & Flack, 1976) and NRC system of programs (Ahmed, Hall, Pippy & Huber, 1973); IBM 370-145 computer of the Computer Center of the University of Chile.

Discussion. The final positional and isotropic thermal parameters of all atoms are listed in Table 1.* Interatomic distances and bond angles are given in Table 2. Fig. 1 shows the thermal ellipsoids, and atom notation.

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* Lists of structure factors, anisotropic thermal parameters, H-atom coordinates and least-squares-planes' data have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 38677 (17 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. *Fractional atomic coordinates ($\times 10^4$) and equivalent isotropic U values (Å$^2 \times 10^3$) with e.s.d.'s in parentheses*

$$U_{eq} = (U_{11} + U_{22}\sin^2\beta + U_{33} + 2U_{13}\cos\beta)/3\sin^2\beta.$$

	x	y	z	U_{eq}
N(1)	2858 (7)	4994 (9)	5172 (5)	45 (3)
N(2)	2019 (6)	6384 (9)	6102 (5)	45 (4)
O	3788 (5)	3737 (7)	4099 (4)	55 (3)
C(1)	1405 (8)	4565 (10)	3267 (6)	41 (4)
C(2)	2493 (8)	3895 (10)	3224 (6)	45 (4)
C(3)	2207 (9)	3349 (11)	2240 (7)	50 (5)
C(4)	0900 (10)	3527 (13)	1311 (7)	57 (5)
C(5)	−0163 (9)	4210 (13)	1353 (6)	58 (5)
C(6)	0077 (8)	4740 (12)	2312 (6)	52 (4)·
C(7)	1656 (9)	5053 (10)	4294 (7)	43 (4)
C(8)	3036 (8)	5542 (11)	6140 (6)	40 (4)
C(9)	4293 (8)	5120 (10)	7084 (6)	45 (5)
C(10)	4547 (8)	5582 (10)	8071 (6)	45 (4)
C(11)	3492 (9)	6480 (11)	8037 (7)	51 (5)
C(12)	2275 (8)	6849 (11)	7053 (7)	52 (5)
C(13)	5876 (9)	5118 (13)	9124 (7)	66 (5)
H	3923 (59)	4087 (84)	4632 (49)	55*

* U_{iso}.

Table 2. *Bond lengths (Å) and bond angles (°) with e.s.d.'s in parentheses*

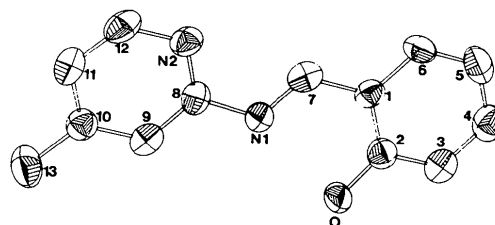|			
C(1)–C(2)	1.41 (2)	C(7)–N(1)	1.27 (1)
C(2)–O	1.34 (1)	N(1)–C(8)	1.42 (1)
O–H	0.78 (8)	C(8)–C(9)	1.38 (1)
C(2)–C(3)	1.39 (1)	C(9)–C(10)	1.39 (1)
C(3)–C(4)	1.38 (1)	C(10)–C(13)	1.50 (1)
C(4)–C(5)	1.39 (2)	C(10)–C(11)	1.39 (2)
C(5)–C(6)	1.37 (1)	C(11)–C(12)	1.38 (1)
C(6)–C(1)	1.40 (1)	C(12)–N(2)	1.34 (1)
C(1)–C(7)	1.46 (2)	N(2)–C(8)	1.33 (1)
C(2)–C(1)–C(6)	119.4 (9)	C(7)–N(1)–C(8)	119.2 (9)
C(1)–C(2)–C(3)	119.1 (7)	N(1)–C(8)–C(9)	116.1 (9)
C(3)–C(2)–O	118.5 (9)	N(1)–C(8)–N(2)	119.9 (6)
C(1)–C(2)–O	122.4 (8)	C(9)–C(8)–N(2)	124.0 (9)
C(2)–O–H	116.3 (45)	C(8)–N(2)–C(12)	115.9 (6)
C(2)–C(3)–C(4)	120.9 (10)	N(2)–C(12)–C(11)	124.3 (10)
C(3)–C(4)–C(5)	119.9 (9)	C(12)–C(11)–C(10)	119.5 (10)
C(4)–C(5)–C(6)	120.8 (7)	C(11)–C(10)–C(9)	116.4 (6)
C(5)–C(6)–C(1)	119.9 (10)	C(11)–C(10)–C(13)	121.2 (9)
C(7)–C(1)–C(2)	120.4 (6)	C(9)–C(10)–C(13)	122.4 (9)
C(7)–C(1)–C(6)	120.3 (9)	C(10)–C(9)–C(8)	119.9 (9)
C(1)–C(7)–N(1)	122.2 (10)		

Fig. 1. Molecule showing atomic labelling, and 50% probability thermal ellipsoids. The omitted H atoms have the same numbering as the parent atoms.

The C–C bond distances in the salicylidene ring are in the range 1.37 (1) to 1.41 (2) Å, comparable with those found in similar Schiff bases (Moustakali-Mavridis, Hadjoudis & Mavridis, 1978, 1980). An intramolecular O–H···N(1) hydrogen bond is observed in the salicylidene group, where N(1)···H is 1.97 (9) Å, N(1)···O is 2.60 (1) Å and O–H···N(1) is 139 (5)°.

C(7)–N(1) is 1.27 (1) Å. C=N double bonds ranging from 1.258 (4) to 1.279 (4) Å have been observed in differently substituted benzylideneanilines (Nakai, Shiro, Ezumi, Sakata & Kubota, 1976; Bar & Bernstein, 1977).

The pyridine ring has C–C distances in the range 1.38 (1) to 1.39 (2) Å, and C–N lengths of 1.34 (1) and 1.33 (1) Å. These distances and the endocyclic angles are comparable with those found in 4-(2,4-dinitrobenzyl)pyridine (Ottersen & Seff, 1974) and in several N-salicylidene-2-aminopyridine [2-(2-pyridyliminomethyl)phenol] derivatives (Moustakali-Mavridis, Hadjoudis & Mavridis, 1978).

Planarity is indicated for the phenyl ring (plane 1), pyridine ring (plane 2) and the plane through C(1), C(2), C(7), O, N(1) (plane 3). Their corresponding χ^2

$[=\sum(\Delta/\sigma)^2]$ values are 5·9, 1·6 and 12·0, respectively. The dihedral angle between the pyridine and phenyl rings is 9·4 (9)°; between the pyridine ring and plane 3 it is 10·7 (9)°. Similar values were also observed in N-salicylidene-3-aminopyridine [2-(3-pyridylimino-methyl)phenol] (Moustakali-Mavridis, Hadjoudis & Mavridis, 1980), where the corresponding dihedral angles were 14·8 and 14·2° respectively.

The deformation of the molecule can be seen from the torsion angles C(1)–C(7)–N(1)–C(8) = 178·0 (8), C(7)–N(1)–C(8)–C(9) = 167·6 (9) and C(7)–N(1)–C(8)–N(2) = −11·4 (13)°. The latter two values show that the pyridine ring is rotated by ~12° about N(1)–C(8) relative to the rest of the molecule, as observed in N-salicylidene-3-aminopyridine. In the latter case, H(7) and the corresponding H of the C atom that substitutes N(2) are located at a distance less than the van der Waals radii. This fact was used to explain the observed deformation, since steric hindrance was supposed to exist. However, in the present compound N(2) is cis to H(7) and there is no possibility for H···H steric hindrance. Since some authors claim that there is a relation between the photochromic properties of a compound and its planarity (Moustakali-Mavridis, Hadjoudis & Mavridis, 1978), studies of these properties will be undertaken in this case.

Fig. 2 shows the projection of the structure onto the xz plane, revealing some of the shortest intermolecular distances. These indicate that the packing in the crystal is due only to van der Waals interactions.
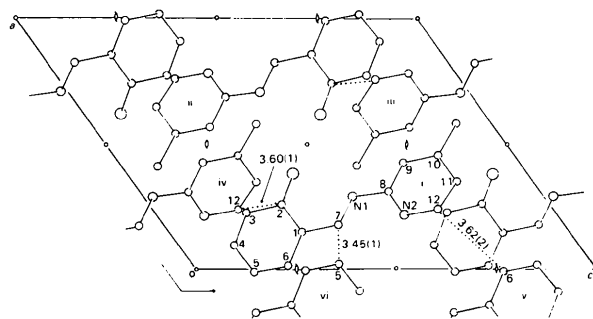
Fig. 2. Structure as viewed along the b axis. The shortest intermolecular distances (Å) are shown. Symmetry code: (i) x,y,z; (ii) $-x, -y, -z$; (iii) $1-x, 1-y, 1-z$; (iv) $x, \frac{3}{2}-y, -\frac{1}{2}+z$; (v) $x, 1-y, 1-z$; (vi) $-x, \frac{1}{2}+y, \frac{1}{2}-z$.

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Structure Refinement of 1,2,3-Triaminoguanidinium Chloride, $CH_9N_6^+.Cl^-$

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Abstract. $M_r = 140·57$, $P6_3/m$, $a = 7·480$ (1), $c = 6·218$ (1) Å, $V = 301·3$ Å³, $Z = 2$, $D_m = 1·550$, $D_x = 1·549$ Mg m⁻³, Cu $K\alpha$, $\lambda = 1·54184$ Å, $\mu = 4·92$ mm⁻¹, $F(000) = 148$, $T = 296$ (1) K, $R = 0·049$, 280 unique reflections. The crystal structure consists of layers of ions parallel to (001) at $\pm \frac{1}{4}c$. Each Cl⁻ anion is hydrogen bonded to three triaminoguanidinium cations within each layer. Only the guanidinium H atoms form