

(Kanters, Roelofsen & Smits, 1977), and a very small number of their acyclic derivatives, e.g. D-dibromomannitol (Simon & Sasvari, 1973) have been reported. A tetraacetate cyclic derivative of D-mannitol has also been reported (Cameron, Cordes & Grindley, 1977). The detailed conformation of the title compound is determined primarily by steric and stereoelectronic (Bürgi, Dunitz & Shefter, 1974) intramolecular interactions between the carbomethoxy substituents.

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## Structure of 2-[(3-Nitrophenylimino)methyl]phenol

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**Abstract.** C<sub>13</sub>H<sub>10</sub>N<sub>2</sub>O<sub>3</sub>,  $M_r = 242.23$ , orthorhombic,  $Pca2_1$ ,  $a = 26.579$  (2),  $b = 3.946$  (4),  $c = 10.756$  (2) Å,  $V = 1128.1$  (1) Å<sup>3</sup>,  $Z = 4$ ,  $D_x = 1.426$  Mg m<sup>-3</sup>,  $\lambda(\text{Mo } K\alpha) = 0.71069$  Å,  $\mu = 0.10$  mm<sup>-1</sup>,  $F(000) = 504$ ,  $T = 298$  K,  $R = 0.0731$  for 985 observed reflections [ $I > 2.5\sigma(I)$ ]. The two phenyl rings are rotated slightly about C—N with a torsion angle of 6.6 (2)°. The C—N distance [1.281 (8) Å] is indicative of a double bond while the N atom is intramolecularly hydrogen bonded to the hydroxyl group with N⋯H = 1.8 (1) Å and N⋯O 2.657 (9) Å.

**Experimental.** The *N*-(3-nitrophenyl)salicylideneamine was prepared by a previously reported method

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(Srivastava & Chauhan, 1977). Preliminary data obtained from Weissenberg and Buerger precession photographs yielded approximate cell dimensions and showed orthorhombic symmetry, space group  $Pca2_1$  or  $Pcam$  from systematic absences  $0kl$ ,  $l = 2n + 1$ ;  $h0l$ ,  $h = 2n + 1$ . Data collection on a crystal  $0.3 \times 0.2 \times 0.2$  mm was performed on a  $P2_1$  diffractometer in  $2\theta/\theta$  mode ( $0 < h < 26$ ,  $0 < k < 4$ ,  $0 < l < 13$ ) to  $2\theta_{\max}$  of 52.0°. Variable scan speed of 5.0–29.3° min<sup>-1</sup> was used. Lattice parameters refined using 30 reflections in the range  $25 < 2\theta < 35^\circ$ . Standard reflection (4 $\bar{1}$ 2) checked every 50 reflections: no significant deviation. The data were corrected for Lorentz and polarization effects. 1384 reflections were collected, 1186 unique ( $R_{\text{int}} = 0$ ), of which 985 observed reflections with  $I > 2.5\sigma(I)$  were

Table 1. Atomic coordinates ( $\times 10^4$ ) and  $B_{\text{eq}}$  ( $\text{\AA}^2$ ) values for non-hydrogen atoms with *e.s.d.*'s in parentheses

	$B_{\text{eq}} = 8\pi^2(U_{11} + U_{22} + U_{33})/3.$			
	x	y	z	$B_{\text{eq}}$
C1	4670 (2)	2620 (13)	2847	3.6 (2)
C2	4512 (2)	1049 (14)	3954 (7)	3.9 (2)
C3	4019 (3)	11 (16)	4086 (7)	4.7 (3)
C4	3666 (3)	661 (16)	3159 (8)	5.1 (3)
C5	3813 (2)	2284 (15)	2080 (8)	4.5 (3)
C6	4314 (2)	3208 (15)	1922 (7)	4.3 (3)
O1	4839 (2)	417 (14)	4891 (6)	5.6 (2)
C7	5187 (2)	3621 (14)	2634 (7)	4.1 (3)
N1	5535 (2)	3216 (12)	3445 (7)	4.1 (2)
C8	6043 (2)	4213 (14)	3189 (7)	3.7 (2)
C9	6406 (2)	3239 (15)	4060 (7)	3.9 (3)
C10	6898 (2)	4046 (17)	3829 (8)	4.4 (3)
C11	7058 (2)	5768 (17)	2776 (8)	5.0 (3)
C12	6696 (3)	6775 (17)	1936 (8)	5.4 (3)
C13	6200 (3)	5993 (15)	2115 (8)	4.8 (3)
N2	7286 (3)	2883 (18)	4742 (7)	5.8 (3)
O2	7727 (3)	3593 (20)	4521 (8)	8.3 (4)
O3	7138 (2)	1331 (18)	5652 (7)	7.9 (3)

Table 2. Bond distances ( $\text{\AA}$ ) and angles ( $^\circ$ ) with *e.s.d.*'s in parentheses for non-hydrogen atoms

C2—C1	1.407 (8)	C6—C1—C2	118.4 (5)
C6—C1	1.391 (8)	C7—C1—C2	122.5 (5)
C7—C1	1.448 (8)	C7—C1—C6	119.1 (5)
C3—C2	1.381 (9)	C3—C2—C1	120.1 (5)
O1—C2	1.355 (7)	O1—C2—C1	121.2 (5)
C4—C3	1.392 (9)	O1—C2—C3	118.6 (5)
C5—C4	1.382 (10)	C4—C3—C2	120.7 (6)
C6—C5	1.392 (8)	C5—C4—C3	119.8 (6)
N1—C7	1.281 (8)	C6—C5—C4	119.6 (6)
C8—N1	1.434 (7)	C5—C6—C1	121.3 (6)
C9—C8	1.397 (8)	N1—C7—C1	122.9 (5)
C13—C8	1.415 (8)	C8—N1—C7	121.0 (5)
C10—C9	1.370 (8)	C9—C8—N1	116.4 (5)
C11—C10	1.388 (9)	C13—C8—N1	124.8 (5)
N2—C10	1.496 (9)	C13—C8—C9	118.7 (5)
C12—C11	1.380 (10)	C10—C9—C8	118.3 (6)
C13—C12	1.366 (10)	C11—C10—C9	123.7 (6)
O2—N2	1.228 (8)	N2—C10—C9	118.0 (6)
O3—N2	1.220 (9)	N2—C10—C11	118.3 (6)
		C12—C11—C10	117.5 (6)
		C13—C12—C11	121.1 (7)
		C12—C13—C8	120.7 (6)
		O2—N2—C10	117.4 (7)
		O3—N2—C10	117.2 (7)
		O3—N2—O2	125.4 (7)

used for refinement of the structure. Structure solved by direct methods, *SHELXS86* (Sheldrick, 1986) and refined using *SHELX76* (Sheldrick, 1976). Scattering factors for C, H, N, O inlaid in *SHELX76*. Space group *Pca2*<sub>1</sub> confirmed from successful solution and refinement of structure.

Structure determination and refinement performed on IBM 4361/4381. Refinement by full-matrix least squares based on *F* with idealized riding H atoms (C—H 0.96  $\text{\AA}$ ) except hydroxyl H which was located from difference map and refined; anisotropic refinement of non-H atoms, individual isotropic *U*'s for H; no absorption correction. In the final cycle, 24 reflections for which  $|F_o - F_c| > 4\sigma(F_o)$  were omitted. The final agreement factors were  $R = 0.0731$ .  $wR = 0.0792$ . Weight for every observed structure factor calculated according to  $w = 15.7559/[\sigma^2(F) + 0.000107F^2]$ ,  $(\Delta/\sigma)_{\text{max}} = 0.015$ ,  $\Delta\rho_{\text{max}} = 0.223$  and  $\Delta\rho_{\text{min}} = -0.238 \text{ e \AA}^{-3}$ . Geometrical calculations performed with *XANADU* (Roberts & Sheldrick, 1975) and illustrations drawn with *ORTEP* (Johnson, 1965). The atomic parameters for non-H atoms are given in Table 1.\* Table 2 contains bond distances and angles, while the atom-labelling scheme is shown in Fig. 1.

**Related literature.** The coordinative behaviour of the Schiff base, *N*-(3-nitrophenyl)salicylideneamine, generated by condensing salicylaldehyde with 3-

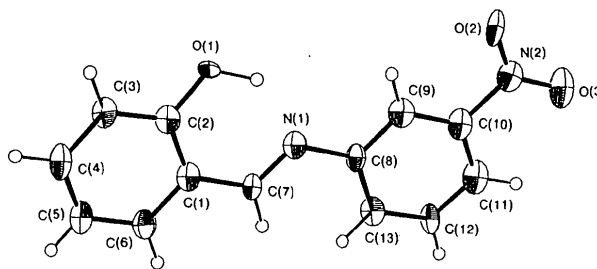


Fig. 1. A perspective view of the molecule.

nitroaniline, is well known but it has only been characterized spectroscopically (Srivastava & Chauhan, 1977; Dwivedi, Bhatnagar & Srivastava, 1986).

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\* Tables of anisotropic thermal parameters, H-atom parameters, distances and angles involving H atoms, and the observed and calculated structure amplitudes have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 54744 (19 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.