hydrogen-bonding distances of 2·86 and 2·81 Å respectively from $O(4)[\bar{1} - x, -\frac{1}{2} + y, \bar{1} - z]$ and $O(3')[2 - x, y + \frac{1}{2}, 1 - z]$ and is possibly hydrogen bonded to them [$O(4)\cdots OW\cdots O(3')$, 134°], but the location of the H atoms of the water is not unequivocal. Around the water O atom, two diffuse clouds of electron density (of approximately 0·3 e Å^{-3} extending up to 1 Å in the **b** direction) are present. If these densities are taken to represent the two H atoms of the water molecule and their coordinates are refined, their new orientations do not correspond to the possible hydrogen bonding involving O(3') and O(4).

• The intercalation of water between nucleic acid bases (Fig. 4) is very unusual (Srikrishnan & Parthasarathy, 1976). It is interesting to note that 5-nitrouridine monohydrate (Egert, Lindner, Hillen & Gassen, 1977) does not form a water sandwich. The water molecules are found to be nearly in the plane of nucleic acid bases (Fig. 2), as found in other related structures. In addition, they intercalate between bases in one stack of nucleic acid bases but are in the same plane as the nucleic acid bases in an adjacent stack, that is shifted, vertically relative to the first stack, by approximately 3·2 Å.

The occurrence of a $C(sp^2)-H\cdots O$ hydrogen bond (Table 3) [$C(6)-HC(6)\cdots O(5')$] in this structure is noteworthy. The presence of an 'electron-withdrawing' nitro group adjacent to C(6)–H causes additional polarization of this bond and enables this H to take part in a hydrogen bond. In addition, there are three $C(sp^3)-H\cdots O$ interactions (Table 3) involving the ribose C atoms. These interactions are unexpected since these contacts involve $C(sp^3)-H$ and not $C(sp^2)-H$ bonds.

The contacts from H(C2') and H(C4') (Table 3) are of the order of the sum of the van der Waals radii of H

and O. The distances and angles involved (Table 3) indicated some attractive interaction between the $C(sp^3)-H$ and the potential hydrogen-bond acceptors.

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The Structure of *p*-Dimethylaminobenzoic Acid

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Abstract. $C_9H_{11}NO_2$, triclinic, $P\bar{1}$, $a = 8·598$ (7), $b = 8·061$ (7), $c = 6·652$ (8) Å; $\alpha = 66·099$ (6), $\beta = 94·62$ (5), $\gamma = 90·97$ (5)°, $D_m = 1·29$, $D_x = 1·31$ g cm^{-3}, $Z = 2$. The structure was determined from three-dimensional X-ray diffraction data and refined by the least-squares method to $R = 0·113$. The dimethyl-amino and carboxyl groups are displaced slightly from the plane of the benzene ring and the N atom is non-planar. Pairs of molecules link together to form dimers through two $O-H\cdots O$ hydrogen bonds (2·622 Å) and the N atom is free from any binding of either type $N-H\cdots O$ or $N-H\cdots C$.

Introduction. The structures of several benzoic acid derivatives have been studied recently with considerable accuracy (Domenicano, Vaciago & Coulson, 1975). The structures of p-toluic acid (Barve & Pant, 1971), p-nitrobenzoic acid (Sakore & Pant, 1966) and p-aminobenzoic acid (Lai & Marsh, 1967) were determined to study the effect of para-substituents on the aromatic-ring moiety.

The structure of p-dimethylaminobenzoic acid (hereinafter, PDBA), with the dimethylamino group as a para-substituent having relatively intermediate behaviour as compared with the nitro and amino groups, is expected to yield more information about the co-operative electronic interaction in the para-substituted compounds.

The crystals were obtained from a water–alcohol mixture. Intensity data were collected on a Picker four-circle computer-controlled X-ray diffractometer with Ni-filtered Cu $K\alpha$ radiation. The intensities of 1147 non-zero reflections were corrected for the Lorentz–polarization factor; absorption correction was neglected.

Possible trial structures in the (001) projection were postulated, assuming planar centrosymmetrical dimers of PDBA with standard bond lengths and angles. The Fourier maps of these trial structures were obtained

and it was found possible to choose a correct trial structure with the help of sets of strong reflections of type $(hh0)$ and $(hh0)$. The trial structure was then refined to $R = 0.32$ by two-dimensional Fourier and difference Fourier methods.

The z parameters were determined from stereo-chemical considerations. The approximate parameters thus obtained gave $R = 0.49$ for three-dimensional data. Successive Fourier and difference Fourier synthesis improved the structure to $R = 0.21$. For initial calculations, an average temperature factor of 2.5 Å² and atomic scattering factors calculated from the analytical constants of Moore (1963) were used.

Table 3. Least-squares planes

(a) Equations of least-squares planes, where X, Y, Z are orthogonal coordinates (Å) referred to crystallographic a, b, c^* axes

Plane 1: benzene ring
$$0.74047X + 0.53652Y + 0.40478Z + 3.49397 = 0.0$$

Plane 2: C(1), C(2), O(1), O(2)
$$0.71040X + 0.59430Y + 0.37701Z + 3.5281 = 0.0$$

Plane 3: C(5), N, C(8), C(9)
$$0.69870X + 0.58495Y + 0.41190Z + 3.50627 = 0.0$$

(b) Deviations (Å) of atoms from planes

	Plane 1	Plane 2	Plane 3
C(1)	+0.0091	–	+0.1444
C(2)	−0.0017	+0.0003	+0.0960
C(3)	0.0	−0.0703	+0.0083
C(4)	+0.0032	−0.0548	−0.0256
C(5)	−0.0046	+0.0299	+0.0018
C(6)	+0.0030	+0.1157	+0.1170
C(7)	+0.0002	+0.0973	+0.1490
C(8)	+0.1063	+0.0737	–
C(9)	−0.0390	+0.1023	–
N	+0.0134	+0.0608	–
O(1)	+0.0913	–	+0.1790
O(2)	−0.0634	–	+0.1540

Table 1. Fractional coordinates ($\times 10^4$), with their standard deviations in parentheses

	x	y	z
C(1)	901 (5)	982 (6)	7208 (8)
C(2)	1576 (5)	1711 (6)	5062 (7)
C(3)	2588 (6)	627 (7)	4553 (9)
C(4)	3248 (7)	1265 (7)	2564 (9)
C(5)	2913 (6)	3054 (7)	985 (8)
C(6)	1897 (6)	4161 (7)	1521 (8)
C(7)	1247 (6)	3463 (7)	3545 (8)
C(8)	4715 (8)	2638 (9)	8571 (10)
C(9)	3211 (7)	5517 (8)	7356 (9)
N	3585 (6)	3715 (6)	9009 (7)
O(1)	1288 (5)	9435 (5)	8612 (6)
O(2)	9920 (4)	1987 (5)	7573 (6)

Table 2. Atomic parameters of the hydrogen atoms from the difference Fourier map

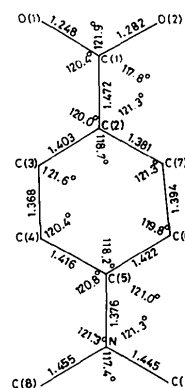|	x	y	z
H(C3)	0.30	−0.06	0.58
H(C4)	0.42	0.08	0.26
H(C6)	0.16	0.52	0.04
H(C7)	0.08	0.42	0.42
H(C81)	0.39	0.19	−0.18
H(C82)	−0.16	0.10	0.00
H(C83)	−0.46	0.26	−0.14
H(C91)	−0.16	0.10	0.00
H(C92)	0.21	0.46	−0.30
H(C93)	0.42	0.08	0.26
H(O2)	−0.40	0.14	0.0

Fig. 1. Bond lengths (Å) and angles.

Two rounds (of four cycles each) of full-matrix least-squares refinement with anisotropic thermal parameters and extinction correction reduced the final R value to 0·113; the use of a weighting scheme (Cruickshank & Dana, 1961) accelerated the convergence. The final atomic positional parameters are given in Table 1. The H atom positions (Table 2), obtained from a difference Fourier map, were included in the final F_c calculations with $B = 4·5 \text{ Å}^2$, but there was no improvement in R.*

Discussion. The equations of planes through the benzene ring (plane 1), carboxyl group (plane 2) and dimethylamino group (plane 3) along with the deviations of different atoms are given in Table 3. In the molecule, C(1) and N are displaced by 0·009 and 0·013 Å, respectively, from plane 1, while the substituent dimethylamino and carboxyl groups are displaced significantly from this plane. The dihedral angles between planes 1 and 2, and planes 2 and 3 are 4·0 and 2·2° respectively. The intramolecular bond

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* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 33212 (4 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

Table 4. *Intermolecular distances* (Å)

N···C(1ⁱ)	3·624	N···C(5ⁱⁱ)	3·951
N···C(2ⁱ)	3·884	N···C(9ⁱⁱ)	3·726
N···O(1ⁱ)	4·038	O(1)···C(8ⁱⁱⁱ)	3·875
N···O(2ⁱ)	3·637	*O(1)···O(2ⁱᵛ)	2·622
N···Nⁱⁱ	3·671	O(2)···O(2ᵛ)	3·505

Symmetry code

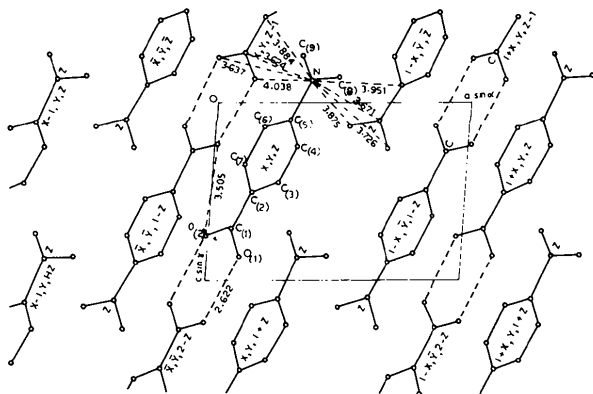|								
(i)		x,	y,	$z - 1$	(iv)	$\bar{x}$,	$\bar{y}$,	$2 - z$
(ii)	$1 - x$,	$1 - y$,	$\bar{z}$		(v)	$\bar{x}$,	$\bar{y}$,	$1 - z$
(iii)		x,	y,	$1 + z$				

* Hydrogen bond.

Fig. 2. Structure projected on (010).

lengths and angles are shown in Fig. 1. The estimated standard deviations (e.s.d.'s) in C—C, C—N and C—O bonds are 0·009, 0·009 and 0·008 Å respectively and the average e.s.d. in bond angles is of the order of 0·6°. The average C—C bond length (1·397 Å) in the aromatic ring is comparable with the values found in crystalline benzene, 1·393 Å (Cox, Cruickshank & Smit, 1958), *p*-nitrobenzoic acid, 1·396 Å (Sakore & Pant, 1966), and *p*-aminobenzoic acid, 1·391 Å (Lai & Marsh, 1967). The exocyclic C(1)—C(2) bond length (1·472 Å) agrees with the expected $C(sp^2)$—$C(sp^2)$ distance and compares with that (1·487 Å) observed in *p*-nitrobenzoic acid. The two C—O bonds (1·248 and 1·282 Å) compare with those observed in other carboxylic acid groups (Leiserowitz, 1976) in a disordered form. The C(5)—N bond length (1·376 Å) is in agreement with the values observed in *p*-nitroaniline (Trueblood, Goldish & Donohue, 1961) and *N*-methylanthranilic acid (Dhaneshwar & Pant, 1972). The N—C(8) and N—C(9) bonds (1·455 and 1·445 Å respectively) are slightly shorter than the expected value for a C—N single bond.

As is typical of carboxylic acids, pairs of molecules form dimers through strong O—H···O-type hydrogen bonds (2·622 Å), as observed in *p*-nitrobenzoic acid (2·65 Å) and in other similar structures. Some of the intermolecular contacts up to about 4·0 Å are shown in Fig. 2 and given in Table 4.

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