Table 1 (*cont.*)

(*b*) Hydrogen atoms ($\times 10^3$)

	x	*y*	*z*
H(1)	−114 (14)	130 (22)	4 (10)
H(3)	−327 (15)	−218 (28)	409 (11)
H(4)	−644 (15)	−305 (28)	350 (11)
H(5)	−743 (15)	−218 (29)	217 (11)
H(6)	−541 (15)	−126 (27)	68 (11)

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The structure of *N*,*N*-dimethylanthranilic acid.*

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The crystals of *N*,*N*-dimethylanthranilic acid, $N(CH_3)_2C_6H_4COOH$, are monoclinic, space group $P2_1/n$ with $a=7{\cdot}66$, $b=15{\cdot}74$, $c=7{\cdot}58$ Å; $\beta=100{\cdot}0°$; ϱ_c for $Z=4$, 1·218 g cm^{-3}. The structure was solved by direct methods with visually estimated data and refined by the method of least squares, resulting in an *R* value of 0·113 for 1037 observed reflexions; the e.s.d.'s in bond lengths not involving hydrogen atoms are 0·006–0·009 Å and in bond angles about 0·5°. The molecule exists in the crystal in the form of a zwitterion. There is a strong intramolecular NH···O hydrogen bond in which the N–O distance is 2·497 Å and O–H distance, 1·42 Å; the angle ONH is 16°.

This work is a continuation of our earlier study of the structure of *N*-methylanthranilic acid (Dhaneshwar & Pant, 1972). The crystals grown from solution in carbon tetrachloride are monoclinic, space group $P2_1/n$ with $a=7{\cdot}66$, $b=15{\cdot}74$, $c=7{\cdot}58$ Å; $\beta=100{\cdot}0°$; ϱ_c for $Z=4$, 1·218 g cm^{-3}. The axial lengths were measured from high-angle reflexions ($\theta\sim75°$) on zero-layer Weissenberg photographs with the films mounted in the Straumanis arrangement; β was determined by the method of triangulation (Jeffery, 1971). Owing to paucity of high-angle reflexions, errors could not be estimated but are expected to be within 0·02 Å in axial lengths and 0·2° in β. The density could not be measured as the crystals are soluble in all common solvents. Data were collected with unfiltered Cu radiation from zero to fourth-layer Weissenberg photographs about the '*a*' axis and from zero to fifth layer photographs about the '*c*' axis; the crystals used for the two sets of photographs had cross-sections $0{\cdot}5\times0{\cdot}6$ mm^2 and $0{\cdot}6\times1{\cdot}2$ mm^2 respectively. The data were processed in the usual way; absorption was neglected.

The normalized values of 157 structure factors were used in the Sayre's-equation program written by Long (1965); signs of 156 *F*'s were obtained and the three-dimensional Fourier map obtained from these revealed all the non-hydrogen atoms. The structure was first refined isotropically with unit weight for all reflexions; later hydrogen atoms and anisotropic temperature factors were included and the refinement continued using Cruickshank's weighting scheme. The final *R* is 0·113 for 1037 observed reflexions. The final atomic and thermal parameters along with their

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Table 1. *Final atomic and thermal parameters and their estimated standard deviations (in parentheses)*

Anisotropic thermal parameters are of the form $T=\exp[-(b_{11}h^2+b_{22}k^2+b_{33}l^2+2b_{12}hk+2b_{23}kl+2b_{13}hl)]$.

(*a*) Non-hydrogen atoms ($\times 10^4$)

	x	*y*	*z*	b_{11}	b_{22}	b_{33}	b_{12}	b_{23}	b_{13}
C(1)	5638 (7)	1227 (3)	3938 (8)	147 (9)	44 (2)	203 (12)	12 (4)	15 (4)	34 (9)
C(2)	7313 (6)	1132 (3)	3455 (7)	141 (9)	47 (3)	133 (10)	7 (4)	3 (4)	26 (8)
C(3)	8792 (7)	1526 (4)	4358 (8)	161 (10)	56 (3)	242 (15)	−9 (4)	−20 (5)	39 (10)
C(4)	8615 (9)	2051 (4)	5824 (9)	244 (14)	62 (3)	233 (14)	−2 (5)	−37 (6)	18 (11)
C(5)	6977 (9)	2155 (4)	6292 (9)	295 (15)	53 (3)	248 (15)	9 (5)	−28 (6)	47 (12)
C(6)	5529 (8)	1748 (4)	5380 (8)	236 (12)	53 (3)	200 (12)	30 (5)	−3 (5)	76 (10)
C(7)	3990 (7)	797 (4)	2896 (8)	116 (9)	56 (3)	261 (15)	6 (4)	20 (5)	48 (9)
C(8)	8457 (8)	−202 (4)	2484 (9)	204 (12)	51 (3)	255 (15)	15 (5)	−14 (5)	59 (11)
C(9)	8202 (10)	1044 (5)	475 (10)	291 (16)	69 (4)	232 (16)	−33 (6)	2 (6)	114 (14)
O(1)	2586 (5)	898 (3)	3482 (6)	155 (7)	87 (3)	315 (12)	0 (3)	2 (5)	92 (8)
O(2)	4167 (5)	398 (3)	1515 (6)	155 (7)	89 (3)	279 (11)	−19 (4)	−57 (5)	28 (7)
N	7449 (5)	588 (3)	1919 (5)	143 (7)	49 (2)	153 (9)	−5 (3)	−13 (4)	51 (6)

Table 1 (*cont.*)

(*b*) Hydrogen atoms ($\times 10^3$)

	x	*y*	*z*
H(1)	992 (9)	146 (5)	418 (9)
H(2)	1009 (10)	238 (5)	633 (10)
H(3)	691 (10)	261 (5)	729 (10)
H(4)	433 (9)	175 (5)	575 (8)
H(5)	595 (8)	58 (4)	136 (8)
H(6)	973 (10)	−1 (5)	306 (10)
H(7)	779 (9)	−45 (5)	340 (9)
H(8)	827 (10)	−59 (5)	132 (10)
H(9)	939 (11)	106 (5)	89 (10)
H(10)	788 (11)	69 (5)	−49 (10)
H(11)	741 (10)	158 (5)	35 (9)

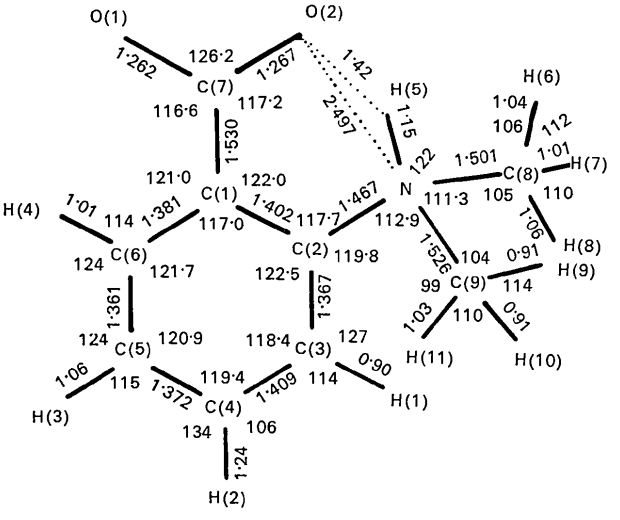

Fig. 1. Bond lengths (Å) and angles (°).

e.s.d.'s (obtained from the diagonal terms of the least-squares inverse matrices) are given in Table 1; F_o and F_c are tabulated by Dhaneshwar (1973).

Table 3. *Equations of planes*

(1) Benzene ring

$$0{\cdot}1801x - 0{\cdot}7837y + 0{\cdot}5945z - 0{\cdot}5794 = 0.$$

(2) Carboxyl group

$$0{\cdot}2004x - 0{\cdot}8281y + 0{\cdot}5236z - 0{\cdot}4258 = 0.$$

Angle between benzene ring and carboxyl group is 4·8°

Deviations of atoms from different planes (Å)

	Planes	
	Benzene ring	Carboxyl group
C(1)	0·002	−0·003
C(2)	−0·003	0·066
C(3)	0·000	
C(4)	0·004	
C(5)	−0·006	
C(6)	0·003	−0·118
C(7)	−0·031	0·010
C(8)	1·270	
C(9)	−1·187	
O(1)	0·029	−0·004
O(2)	−0·151	−0·004
N	−0·017	0·177
H(1)	0·07	
H(2)	−0·09	
H(3)	−0·13	
H(4)	0·09	−0·08
H(5)	−0·34	−0·16
H(6)	1·36	
H(7)	1·95	
H(8)	1·22	
H(9)	−0·95	
H(10)	−1·21	
H(11)	−1·95	

Table 2. *Intramolecular bond lengths and angles*

	Uncorrected	Corrected	E.s.d.		
C(1)–C(2)	1·402 Å		0·007 Å	C(1)—C(2)–C(3)	122·5 (5)°
C(2)–C(3)	1·367		0·008	C(2)—C(3)–C(4)	118·4 (5)
C(3)–C(4)	1·409		0·009	C(3)—C(4)–C(5)	119·4 (6)
C(4)–C(5)	1·372		0·009	C(4)—C(5)–C(6)	120·9 (6)
C(5)–C(6)	1·361		0·009	C(5)—C(6)–C(1)	121·7 (6)
C(6)–C(1)	1·381		0·008	C(6)—C(1)–C(2)	117·0 (5)
C(1)–C(7)	1·526	1·530 Å	0·008	C(7)—C(1)–C(2)	122·0 (5)
C(7)–O(1)	1·243	1·262	0·007	C(7)—C(1)–C(6)	121·0 (5)
C(7)–O(2)	1·248	1·267	0·007	O(1)—C(7)–C(1)	116·6 (5)
C(2)–N	1·464	1·467	0·006	O(2)—C(7)–C(1)	117·2 (5)
C(8)–N	1·487	1·501	0·008	O(1)—C(7)–O(2)	126·2 (6)
C(9)–N	1·505	1·526	0·009	N——C(2)–C(1)	117·7 (4)
C(3)–H(1)	0·90		0·07	N——C(2)–C(3)	119·8 (5)
C(4)–H(2)	1·24		0·08	C(8)—N——C(2)	111·4 (4)
C(5)–H(3)	1·06		0·08	C(9)—N——C(2)	112·9 (4)
C(6)–H(4)	1·01		0·07	C(8)—N——C(9)	111·3 (5)
N——H(5)	1·15		0·06	C(2)—N——H(5)	96
C(8)–H(6)	1·04		0·08	O(2)—N——H(5)	16
C(8)–H(7)	1·01		0·07	N——H(5)–O(2)	152
C(8)–H(8)	1·06		0·08		
C(9)–H(9)	0·91		0·08	N——C(9)–H(10)	102
C(9)–H(10)	0·91		0·08	N——C(8)–H(7)	103
C(9)–H(11)	1·03		0·08	H(11)–C(9)–H(9)	123
N——O(2)	2·497		0·006	H(8)—C(8)–H(6)	120
O(2)–H(5)	1·42		0·06	C(9)—N——H(5)	103

The intramolecular bond lengths and angles are shown in Fig. 1 and listed in Table 2. The corrections to C(1)–C(7), C(7)–O(1), C(7)–O(2), C(2)–N, N–C(8) and N–C(9) bond distances due to librational effects amounted to 0·004, 0·019, 0·019, 0·003, 0·014 and 0·021 Å respectively; the details of the atomic thermal vibration ellipsoids are given by Dhaneshwar (1973). The equations of the planes of the benzene ring and the carboxyl group (referred to the *a'*, *b*, *c* orthogonal axes), the angle between them and the deviations of the atoms from these planes are given in Table 3.

The molecule exists in the crystal in the form of a zwitterion; the $C-N^+H(CH_3)_2$ distance, $1{\cdot}467 \pm 0{\cdot}006$ Å (1·464 Å without correction for librational effects) is a little shorter than the $C-N^+H_3$ distance in the zwitterionic form of anthranilic acid, $1{\cdot}501 \pm 0{\cdot}006$ Å (uncorrected; Brown, 1968). There is a strong intramolecular NH···O hydrogen bond in which the N–O distance is 2·497 Å and O–H distance, 1·42 Å; the angle ONH is 16°. The packing of molecules in the crystal is shown in Fig. 2.

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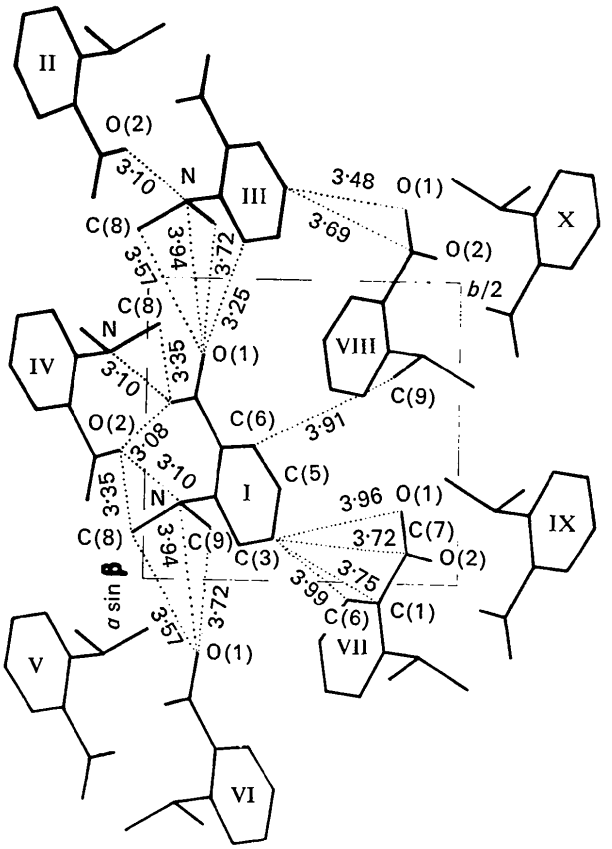

Fig. 2. The (001) projection of the structure, I x,y,z; II $\bar{x},\bar{y},\bar{z}$; III $-1+x,y,z$; IV $1-x,\bar{y},\bar{z}$; V $2-x,\bar{y},\bar{z}$; VI $1+x,y,z$; VII $\frac{1}{2}+x,\frac{1}{2}-y,\frac{1}{2}+z$; VIII $x-\frac{1}{2},\frac{1}{2}-y,\frac{1}{2}+z$; IX $\frac{3}{2}-x,\frac{1}{2}+y,\frac{1}{2}-z$; X $\frac{1}{2}-x,\frac{1}{2}+y,\frac{1}{2}-z$.