SHORT STRUCTURAL PAPERS

Anthranilic Acid II (o-Aminobenzoic Acid)

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Abstract. $C_7H_7NO_2$, space group *Pbca*, $a = 15.973$ (4), $b = 11.605$ (8), $c = 7.162$ (5) Å, $V = 1327.6$ Å^3, $D_x = 1.372$, $D_m = 1.362$ g cm^{-3} (by flotation), $Z = 8$. The final R was 0.059 for 528 counter reflexions and 119 variables. In contrast to anthranilic acid I, all the molecules are in the non-zwitterionic form. They are connected by hydrogen bonds between the carboxyl groups of the cyclic dimer type across centres of symmetry with $O \cdots O = 2.654$ Å, and by $N-H \cdots O$ intermolecular hydrogen bonds with $N \cdots O = 3.122$ Å. The molecules have an intramolecular $N-H \cdots O$ hydrogen bond with $N \cdots O = 2.682$ Å.

Introduction. Anthranilic acid exists in three modifications (McCrone, Whitney & Corvin, 1949). Brown (1968) solved the structure of the low-temperature form I, which is stable up to 81 °C (Arnold & Jones, 1972). Above this temperature the structure changes into modification II.

Thin yellow needles of the title compound were obtained from a saturated benzene solution at room temperature. Intensities were measured at room temperature on an Enraf–Nonius CAD-3 diffractometer with the θ–2θ scan technique up to $\theta = 60°$, Cu $K\alpha$ radiation ($\lambda = 1.5418$ Å), Ni filters and a scintillation counter. Systematic absences were found for $hk0$, $h = 2n + 1$; $h0l$, $l = 2n + 1$; $0kl$, $k = 2n + 1$, from which the space group *Pbca* was inferred. Of the 981 independent reflexions, 528 with $I \geq 2\sigma(I)$ were measured, where $\sigma(I)$ is the variance of the intensity on the basis of counting statistics. No corrections for absorption or extinction were made. The structure was

Table 1. *Fractional coordinates for* C, N, O ($\times 10^4$) *and for* H ($\times 10^3$) *together with distances* (δ) *of the atoms to the least-squares plane through the benzene-ring* C *atoms* (Å)

The e.s.d.'s in parentheses refer to the least significant digit(s).

	x	y	z	δ
C(1)	4407 (3)	54 (5)	2614 (8)	−0.042
C(2)	3964 (3)	157 (5)	866 (7)	−0.0103
C(3)	3638 (3)	1209 (6)	301 (8)	0.0130
C(4)	3188 (4)	1331 (6)	−1305 (10)	−0.0088
C(5)	3085 (4)	379 (7)	−2442 (11)	0.0022
C(6)	3401 (4)	−662 (7)	−1968 (8)	0.0001
C(7)	3851 (3)	−809 (5)	−331 (8)	0.0038
N	4139 (4)	−1861 (5)	151 (8)	−0.043
O(1)	4457 (3)	1041 (3)	3565 (7)	−0.052
O(2)	4690 (2)	−834 (3)	3272 (4)	−0.114
H(1)	471 (4)	93 (5)	436 (8)	−0.016
H(2)	375 (2)	190 (3)	122 (6)	0.025
H(3)	293 (3)	209 (4)	−158 (6)	−0.068
H(4)	276 (3)	40 (4)	−349 (6)	−0.062
H(5)	331 (3)	−136 (3)	−275 (6)	−0.032
H(6)	455 (2)	−197 (3)	88 (5)	0.230
H(7)	409 (3)	−233 (4)	−54 (6)	0.009

Table 2. *Bond lengths* (Å) *and angles* (°) *in anthranilic acid* II

The e.s.d.'s in parentheses refer to the least significant digit(s).

C(1)–C(2)	1.443 (8)	C(4)–C(5)–C(6)	121.4 (7)
C(2)–C(3)	1.387 (8)	C(5)–C(6)–C(7)	121.1 (7)
C(3)–C(4)	1.364 (9)	C(6)–C(7)–C(2)	118.6 (6)
C(4)–C(5)	1.383 (11)	C(2)–C(7)–N	121.0 (5)
C(5)–C(6)	1.353 (11)	C(6)–C(7)–N	120.3 (6)
C(6)–C(7)	1.386 (8)	C(7)–N–H(6)	123.6 (2.6)
C(7)–C(2)	1.423 (8)	C(7)–N–H(7)	117.1 (3.7)
C(1)–O(1)	1.336 (7)	C(7)–C(2)–C(1)	121.3 (5)
C(1)–O(2)	1.219 (7)	C(3)–C(2)–C(1)	120.7 (5)
C(7)–N	1.349 (9)	C(2)–C(1)–O(2)	126.0 (5)
C(3)–H(2)	1.05 (4)	C(2)–C(1)–O(1)	113.6 (5)
C(4)–H(3)	1.00 (5)	O(1)–C(1)–O(2)	120.3 (5)
C(5)–H(4)	0.91 (4)	C(1)–O(1)–H(1)	107.1 (4.8)
C(6)–H(5)	1.00 (4)	C(2)–C(3)–H(2)	115.0 (2.2)
N–H(6)	0.84 (4)	C(4)–C(3)–H(2)	122.6 (2.2)
N–H(7)	0.74 (5)	C(3)–C(4)–H(3)	118.6 (2.6)
O(1)–H(1)	0.71 (6)	C(5)–C(4)–H(3)	122.9 (2.6)
N $\cdots$ O(2)	2.682 (7)	C(4)–C(5)–H(4)	122.1 (2.9)
O(1)$\cdots$O(2')	2.654 (6)	C(6)–C(5)–H(4)	116.3 (2.9)
N$\cdots$O(2'')	3.122 (7)	C(5)–C(6)–H(5)	122.0 (2.5)
		C(7)–C(6)–H(5)	116.8 (2.5)
C(7)–C(2)–C(3)	118.0 (5)	N–H(6)–O(2)	118.7 (3.1)
C(2)–C(3)–C(4)	122.4 (6)	O(1)–H(1)–O(2')	171.3 (6.7)
C(3)–C(4)–C(5)	118.4 (7)	N–H(7)–O(2'')	144.6 (4.7)

solved with *MULTAN* (Germain, Main & Woolfson, 1971). Scattering factors were from Cromer & Mann (1968) for C, O and N and from Stewart, Davidson & Simpson (1965) for H. Refinement was by full-matrix least-squares minimization of $\sum w_i(F_o - F_c)^2$, with weights based on $\sigma(I)$. The final R $(= \sum ||F_o| - |F_c||/\sum |F_o|)$ was 0·059; R_w was 0·040. A final difference synthesis showed no peaks higher than 0·27 e Å⁻³.*

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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 32703 (10 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.
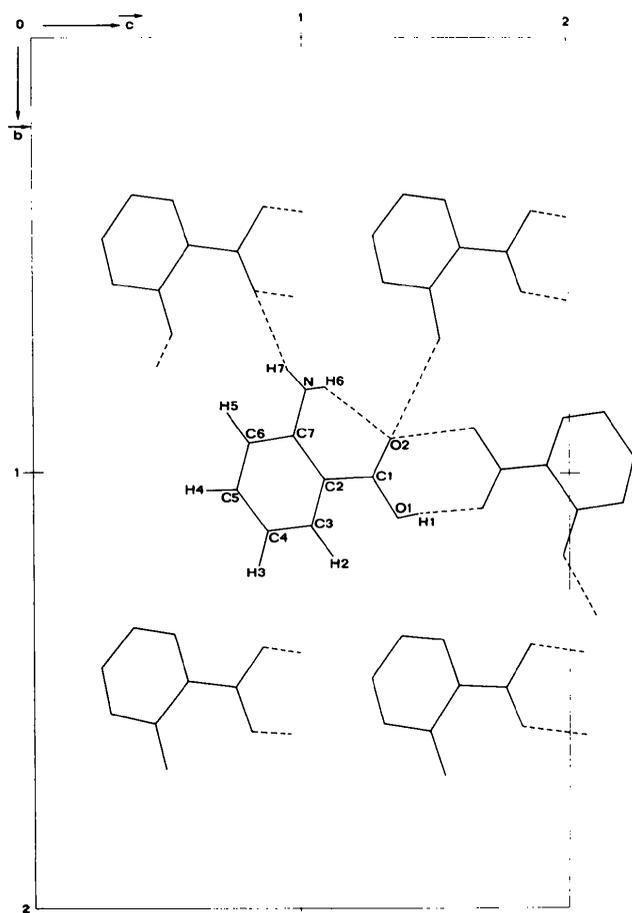
Positional parameters are listed in Table 1, bond lengths and angles in Table 2. All calculations were performed with the XRAY system (1972).

Discussion. This work is part of a programme on intermolecular interactions in hydrogen-bonded molecular crystals. Anthranilic acid, showing polymorphy, is expected to be a suitable compound for investigation as the lattice energies of several modifications may be compared and the effect of zwitterion formation studied.

In anthranilic acid I, Brown (1968) found two different molecules in the asymmetric unit: a neutral molecule and a zwitterion. From the molecular geometry found for anthranilic acid II we conclude that in the second modification all molecules are in the neutral form. The change from (I) to (II) must have important consequences for the electrostatic packing energy; we are now studying these effects quantitatively.

As can be seen in Fig. 1, anthranilic acid II shows the familiar linkage of carboxyl groups by two hydrogen bonds of the cyclic dimer type across centres of symmetry (Leiserowitz, 1976), whereas anthranilic acid I only has single O—H···O hydrogen bonds. In both modifications N—H···O hydrogen bonds connect the molecules into networks, although the rather long N···O distance (3·122 Å) in anthranilic acid II indicates only a weak bond.

The bond lengths and angles show no unexpected features.

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Fig. 1. Projection of the structure down a.

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