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m-Aminobenzoic Acid

BY J. VOOGD, B. H. M. VERZIJL AND A. J. M. DUISENBERG

Department of Structural Chemistry, State University of Utrecht, Padualaan 8, Utrecht, The Netherlands

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Abstract. $C_7H_7NO_2$, $P2_1/c$, $a = 5.047$ (1), $b = 23.060$ (10), $c = 11.790$ (5) Å, $\beta = 105.47$ (3)°, $V = 1322.4$ Å^3, $D_x = 1.376$, $D_m = 1.388$ Mg m^{-3} (by flotation), $Z = 8$; final $R = 0.047$ for 999 reflexions and 223 variables. Like anthranilic acid II (*o*-aminobenzoic acid) and *p*-aminobenzoic acid the molecules are all in the non-zwitterionic form; however, in this case the carboxylic group is somewhat disordered. The molecules are connected by hydrogen bonds between the carboxyl groups of the two different molecules in the asymmetric unit, and are of the cyclic dimer type, with O···O bonds of 2.604 and 2.676 Å. There is one N—H···O hydrogen bond with N···O = 3.146 Å.

Introduction. Thin brownish plates of *m*-aminobenzoic acid were obtained by evaporation of a saturated chloroform solution.

Systematic absences were found on Weissenberg photographs for $0k0$, $k = 2n + 1$ and for $h0l$, $l = 2n + 1$ reflexions, from which the space group $P2_1/c$ was determined. All dimensions and intensities were measured at room temperature on an Enraf–Nonius CAD-4 diffractometer and the ω–2θ scan technique up to $\theta = 27.5°$, Mo $K\alpha$ radiation ($\lambda = 0.71069$ Å), Zr filters and a scintillation counter. Of the 3051 independent reflexions measured, 999 had $I \geq 2\sigma(I)$ and were included in the refinement, 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 solved with *MULTAN* 78 (Main, Hull, Lessinger, Germain, Declercq & Woolfson, 1978). 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 $\sigma^{-2}(F_o)$. The final R was 0.047 ($R = \sum ||F_o| - |F_c||/\sum |F_o|$); R_w was 0.032. A final difference synthesis showed no peaks >0.25 e Å^{-3}.*

* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 35403 (24 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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) *and the equivalent isotropic temperature factors* (Å^2) *for the non-hydrogen atoms*

The e.s.d.'s in parentheses refer to the least significant digit. The e.s.d.'s of δ are for molecule A 0.005 and for molecule B 0.007 Å.

	x	y	z	δ	B_{eq}
Molecule A					
N(1)	−4889 (6)	−537 (2)	4038 (3)	−0.057	4.5 (2)
O(1)	1498 (4)	1113 (1)	3602 (2)	−0.056	4.1 (1)
O(2)	−419 (5)	1424 (1)	1778 (2)	0.060	4.7 (1)
C(1)	−329 (6)	1085 (2)	2645 (3)	0.005	3.3 (2)
C(2)	−2539 (6)	645 (2)	2442 (3)	0.0019	3.0 (1)
C(3)	−2696 (6)	270 (2)	3340 (3)	−0.0022	3.1 (2)
C(4)	−4771 (6)	−146 (2)	3167 (3)	0.0011	3.2 (2)
C(5)	−6671 (6)	−177 (2)	2063 (3)	0.0004	4.2 (2)
C(6)	−6474 (7)	195 (2)	1188 (3)	−0.0008	5.2 (2)
C(7)	−4430 (7)	607 (2)	1358 (3)	−0.0004	4.3 (2)
H(1)	121 (5)	169 (2)	191 (2)	−0.038	
H(2)	−144 (5)	33 (2)	411 (2)	0.078	
H(3)	−399 (6)	−47 (2)	475 (3)	0.129	
H(4)	−651 (5)	−73 (2)	393 (3)	0.165	
H(5)	−805 (6)	−46 (2)	195 (3)	−0.002	
H(6)	−779 (5)	18 (2)	42 (3)	0.003	
H(7)	−431 (5)	86 (2)	72 (3)	−0.013	
Molecule B					
N(1)	9861 (5)	3664 (2)	1078 (3)	0.030	3.6 (1)
O(1)	3592 (4)	2164 (1)	2021 (2)	0.120	4.0 (1)
O(2)	5550 (4)	1890 (1)	3861 (2)	−0.176	4.1 (1)
C(1)	5440 (6)	2212 (2)	2958 (3)	−0.013	3.0 (2)
C(2)	7635 (6)	2649 (2)	3046 (3)	−0.0031	2.7 (2)
C(3)	7743 (6)	2949 (2)	2045 (3)	0.0079	2.9 (2)
C(4)	9786 (6)	3353 (2)	2084 (3)	−0.0072	2.9 (2)
C(5)	11696 (6)	3465 (2)	3152 (3)	0.0017	3.6 (2)
C(6)	11561 (7)	3168 (2)	4147 (3)	0.0031	4.6 (2)
C(7)	9553 (7)	2758 (2)	4114 (3)	0.0024	3.8 (2)
H(1)	405 (5)	164 (1)	373 (2)	−0.146	
H(2)	636 (6)	288 (1)	132 (3)	0.049	
H(3)	896 (6)	351 (2)	37 (3)	−0.237	
H(4)	1154 (5)	381 (2)	109 (3)	−0.290	
H(5)	1309 (5)	377 (1)	318 (3)	0.039	
H(6)	1291 (5)	325 (2)	486 (2)	−0.005	
H(7)	945 (5)	256 (2)	478 (2)	0.008	

Positional parameters are listed in Table 1, bond lengths and angles in Table 2. All calculations were performed with the XRAY system (1976).

Discussion. This work is part of a programme on intermolecular interactions in hydrogen-bonded

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Table 2. *Bond lengths* (Å) *and angles* (°)

E.s.d.'s are in parentheses.

	Molecule *A*	Molecule *B*
C(4)–N(1)	1·379 (5)	1·395 (5)
C(1)–O(1)	1·254 (4)	1·246 (4)
C(1)–O(2)	1·277 (4)	1·286 (4)
C(1)–C(2)	1·480 (5)	1·481 (4)
C(2)–C(3)	1·385 (5)	1·381 (4)
C(3)–C(4)	1·395 (5)	1·381 (5)
C(4)–C(5)	1·398 (5)	1·391 (4)
C(5)–C(6)	1·365 (6)	1·375 (5)
C(6)–C(7)	1·378 (6)	1·380 (5)
C(7)–C(2)	1·379 (5)	1·391 (4)
O(2)–H(1)	1·00 (3)	0·94 (3)
C(3)–H(2)	0·97 (3)	0·96 (2)
N(1)–H(3)	0·86 (3)	0·92 (3)
N(1)–H(4)	0·91 (3)	0·91 (3)
C(5)–H(5)	0·93 (3)	0·99 (3)
C(6)–H(6)	0·97 (3)	0·95 (2)
C(7)–H(7)	0·97 (3)	0·93 (3)
N(1,*A*)···O(1′,*A*)	3·146 (7)	
O(1,*A*)···O(2,*B*)	2·676 (5)	
O(2,*A*)···O(1,*B*)	2·604 (6)	
O(1)–C(1)–O(2)	123·3 (3)	122·7 (3)
C(2)–C(1)–O(1)	121·5 (3)	119·4 (3)
C(2)–C(1)–O(2)	115·2 (3)	117·9 (3)
C(1)–C(2)–C(3)	119·9 (3)	118·7 (2)
C(2)–C(3)–C(4)	120·7 (3)	120·6 (3)
C(3)–C(4)–C(5)	118·2 (3)	119·1 (3)
C(4)–C(5)–C(6)	120·1 (3)	120·0 (3)
C(5)–C(6)–C(7)	121·7 (3)	121·4 (3)
C(6)–C(7)–C(2)	118·9 (3)	118·5 (3)
C(7)–C(2)–C(3)	120·3 (3)	120·4 (3)
C(7)–C(2)–C(1)	119·9 (3)	120·9 (3)
C(3)–C(4)–N(1)	121·4 (3)	120·5 (3)
C(5)–C(4)–N(1)	120·3 (3)	120·3 (3)
C(1)–O(2)–H(1)	113·2 (1·4)	111·5 (1·5)
C(2)–C(3)–H(2)	118·2 (1·6)	119·8 (1·7)
C(4)–C(3)–H(2)	120·9 (1·6)	119·5 (1·7)
C(4)–N(1)–H(3)	119·9 (2·1)	117·0 (1·8)
C(4)–N(1)–H(4)	115·0 (1·7)	114·9 (1·6)
C(4)–C(5)–H(5)	117·8 (1·7)	118·2 (1·3)
C(6)–C(5)–H(5)	112·1 (1·7)	121·7 (1·3)
C(5)–C(6)–H(6)	120·2 (1·8)	118·3 (1·7)
C(7)–C(6)–H(6)	118·1 (1·8)	120·3 (1·6)
C(6)–C(7)–H(7)	120·5 (1·5)	121·6 (1·5)
C(2)–C(7)–H(7)	120·6 (1·5)	119·9 (1·5)
O(2,*A*)–H(1,*A*)···O(1,*B*)	173·2 (2·5)	
N(1,*A*)–H(3,*A*)–O(1′,*A*)	133·0 (3·2)	
O(2,*B*)–H(1,*B*)···O(1,*A*)	173·6 (2·9)	

molecular crystals. Now that the structure of *m*-aminobenzoic acid has been solved, the crystal structures (of at least one modification) of all three aminobenzoic acids have been determined. This was necessary to compare the lattice energies of these compounds.

m-Aminobenzoic acid has two independent molecules, *A* and *B*, both non-zwitterions in the asymmetric unit, which form a dimer *A–B*. *p*-Aminobenzoic acid (Lai & Marsh, 1967) also has two non-zwitterionic molecules in the asymmetric unit, but here the dimers are *A–A* and *B–B*. Anthranilic acid I (*o*-aminobenzoic acid) (Brown, 1968) has one zwitterionic and one non-zwitterionic molecule in the asymmetric unit, and finally anthranilic acid II (Boone, Derissen & Schoone, 1977) has only one non-zwitterionic molecule in the asymmetric unit, which forms dimers of the type *A–A*.

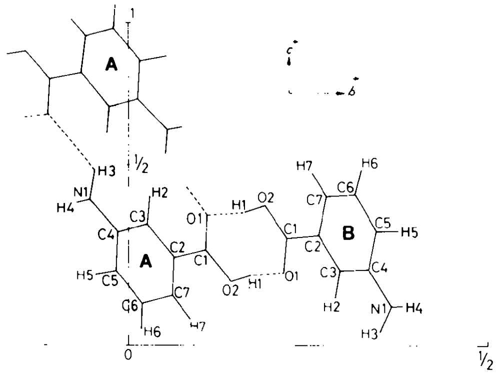

Fig. 1. Projection of the structure along a.

As can be inferred from the bond lengths and angles the carboxyl groups of *m*-aminobenzoic acid are somewhat disordered (Leiserowitz, 1976). Fig. 1 shows the hydrogen-bonding scheme.

Attempts will be made to solve the crystal structure at low temperature.

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