in Table 1 and bond lengths and angles in Table 2.* Fig. 1 shows the structure and atom-labelling scheme.

Related literature. Two other structures are known which contain V—Se bonds: $[(dppe)V(CO)_3]_2Se$ (Albrecht, Hübener, Behren & Weiss, 1985), and V_2Se_9 (Furuseth & Klewe, 1984). The isostructural S analogue has been reported (Bolinger, Rauchfuss & Rheingold, 1982).

* Lists of structure factors, anisotropic thermal parameters and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 43128 (12 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

References

ALBRECHT, N., HÜBENER, P., BEHREN, U. & WEISS, E. (1985). *Chem. Ber.* **118**, 4059–4067.

BOLINGER, C. M., RAUCHFUSS, T. B. & RHEINGOLD, A. L. (1982). *Organometallics*, **1**, 1551–1553.

FORUSETH, S. & KLEWE, B. (1984). *Acta Chem. Scand. Ser. A*, **38**, 467–471.

International Tables for X-ray Crystallography (1974). Vol. IV, pp. 99, 149. Birmingham: Kynoch Press. (Present distributor D. Reidel, Dordrecht.)

SHELDRICK, G. M. (1984). *SHELXTL Program Library*, Version 4.1. Nicolet XRD Corporation, Madison, Wisconsin.

Acta Cryst. (1986). C**42**, 1880–1881

Structure of Monoclinic *o*-Aminobenzoic Acid

BY HIROYUKI TAKAZAWA, SHIGERU OHBA AND YOSHIHIKO SAITO

Department of Chemistry, Faculty of Science and Technology, Keio University, Hiyoshi 3, Kohoku-ku, Yokohama 223, Japan

(*Received* 30 *June* 1986; *accepted* 13 *July* 1986)

Abstract. $C_7H_7NO_2$, $M_r = 137{\cdot}1$, monoclinic, $P2_1/c$, $a = 6{\cdot}537\ (3)$, $b = 15{\cdot}351\ (5)$, $c = 7{\cdot}086\ (3)$ Å, $\beta = 112{\cdot}64\ (3)°$, $V = 656{\cdot}3\ (5)$ Å^3, $Z = 4$, $D_m = 1{\cdot}34\ (1)$, $D_x = 1{\cdot}39$ Mg m^{-3}, $\lambda(\text{Mo } K\alpha) = 0{\cdot}71073$ Å, $\mu = 0{\cdot}097$ mm^{-1}, $F(000) = 288$, $T = 298\ (1)$ K, final $R = 0{\cdot}039$ for 1187 unique reflections. The molecule is non-zwitterionic. The adjacent molecules form a cyclic dimer by intermolecular hydrogen bonds with their carboxyl groups, the O···O distance being 2·651 (3) Å. One of the amino H atoms takes part in an intramolecular hydrogen bond with N···O distance 2·688 (4) Å and the other in a weak intermolecular hydrogen bond with N···O distance 3·385 (5) Å.

Experimental. Colorless prisms of the title compound occasionally grew from an aqueous solution in which O_2 gas was bubbled by cooling gradually from 343 to 313 K. D_m determined by flotation in an aqueous solution of ZnI_2. Crystal size 0·5 × 0·5 × 0·5 mm, Rigaku AFC-5 four-circle diffractometer, Mo $K\alpha$ radiation, graphite monochromator, θ–2θ scan with scan speed 6° min^{-1} in θ, scan width $(1{\cdot}3 + 0{\cdot}5\tan\theta)°$. Range of indices, $-6 \le h \le 6$, $0 \le k \le 14$, $0 \le l \le 6$ $(2\theta \le 55°)$. Lattice constants determined based on 20 2θ values $(20 < 2\theta < 31°)$. Variation of standards <1%; 1618 reflections measured; 1272 observed reflections with $|F_o| > 3\sigma(|F_o|)$. Systematic absences $h0l$, l odd; $0k0$, k odd. No corrections for absorption or extinction. Structure solved by direct methods with *MULTAN*78

Table 1. *Fractional coordinates* (×10^4) *and equivalent isotropic temperature factors* (*Hamilton*, 1959)

$$B_{eq} = \tfrac{1}{3}\sum_i\sum_j B_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	B_{eq}(Å^2 × 10)
C(1)	9484 (2)	4408 (1)	7434 (2)	30
C(2)	9057 (2)	3992 (1)	5459 (2)	29
C(3)	6887 (2)	3982 (1)	3976 (2)	35
C(4)	6388 (3)	3577 (1)	2122 (2)	42
C(5)	8073 (3)	3179 (1)	1710 (2)	45
C(6)	10206 (3)	3187 (1)	3114 (2)	42
C(7)	10780 (2)	3597 (1)	5032 (2)	33
N	12921 (2)	3572 (1)	6407 (2)	45
O(1)	7702 (2)	4708 (1)	7665 (1)	42
O(2)	11336 (2)	4476 (1)	8799 (1)	40

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

C(1)–C(2)	1·465 (2)	C(7)–C(2)–C(3)	119·7 (1)
C(2)–C(3)	1·403 (6)	C(2)–C(3)–C(4)	121·3 (1)
C(3)–C(4)	1·375 (3)	C(3)–C(4)–C(5)	119·1 (1)
C(4)–C(5)	1·385 (3)	C(4)–C(5)–C(6)	120·9 (1)
C(5)–C(6)	1·366 (5)	C(5)–C(6)–C(7)	121·6 (2)
C(6)–C(7)	1·410 (3)	C(6)–C(7)–C(2)	117·4 (1)
C(7)–C(2)	1·411 (3)	C(7)–C(2)–C(1)	121·2 (1)
C(7)–N	1·364 (5)	C(3)–C(2)–C(1)	119·1 (1)
C(1)–O(1)	1·320 (2)	C(6)–C(7)–N	119·7 (1)
C(1)–O(2)	1·229 (5)	C(2)–C(7)–N	122·9 (1)
O(1)···O(2^i)	2·651 (3)	C(2)–C(1)–O(1)	114·7 (1)
N···O(2)	2·688 (4)	C(2)–C(1)–O(2)	123·8 (1)
N···O(1^{ii})	3·385 (5)	O(1)–H(O1)···O(2^i)	173 (2)
		N–H(N)1···O(2)	127 (2)
		N–H(N)2···O(1^{ii})	104 (1)

Symmetry code: (i) $2-x$, $1-y$, $2-z$; (ii) $1+x$, y, z.

0108-2701/86/121880-02$01.50

(Main, Hull, Lessinger, Germain, Declercq & Woolfson, 1978). All the H atoms found from difference synthesis. Non-H atoms refined with anisotropic thermal parameters, and H atoms with isotropic thermal parameters. $\sum w||F_o| - |F_c||^2$ minimized; $w^{-1} = \sigma^2(|F_o|) + (0{\cdot}015|F_o|)^2$. Final $R = 0{\cdot}039$, $wR = 0{\cdot}053$, $S = 1{\cdot}92$ for 1187 unique reflections.* $R_{int} = 0{\cdot}008$. $\Delta/\sigma < 0{\cdot}4$, $-0{\cdot}24 < \Delta\rho < 0{\cdot}17$ e Å^{-3}. Complex neutral-atom scattering factors from *International Tables for X-ray Crystallography* (1974); Universal Crystallographic Computation Program System *UNICS*III (Sakurai & Kobayashi, 1979). Final atomic coordinates are given in Table 1, and bond lengths and angles in Table 2.

Related literature. Two kinds of orthorhombic crystals of *o*-aminobenzoic acid grow in different conditions (Brown, 1968). Brown (1968) and Brown & Ehrenberg (1985) reported a lower-temperature form of the compound which contains a zwitterion, and Boone, Derissen & Schoone (1977) reported a higher-temperature form. The hydrogen-bonding scheme in the present crystal (Fig. 1) is almost the same as that in the other modifications. The structures of *m*- (Voogd, Verzijl & Duisenberg, 1980) and *p*-aminobenzoic acid (Lai & Marsh, 1967) have also been determined.

* Lists of structure factors, anisotropic thermal parameters, atomic parameters for H atoms, bond lengths and bond angles involving H atoms and distances from the least-squares plane through the benzene ring have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 43242 (13 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

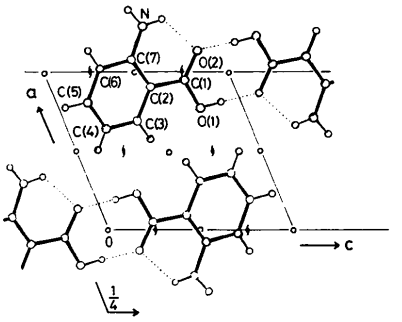

Fig. 1. A partial projection of the structure along **b**. Dotted lines indicate hydrogen bonds.

References

BOONE, C. D. G., DERISSEN, J. L. & SCHOONE, J. C. (1977). *Acta Cryst.* B**33**, 3205–3206.

BROWN, C. J. (1968). *Proc. R. Soc. London Ser. A*, **302**, 185–199.

BROWN, C. J. & EHRENBERG, M. (1985). *Acta cryst.* C**41**, 441–443.

HAMILTON, W. C. (1959). *Acta Cryst.* **12**, 609–610.

International Tables for X-ray Crystallography (1974). Vol. IV. Birmingham: Kynoch Press. (Present distributor D. Reidel, Dordrecht.)

LAI, T. F. & MARSH, R. E. (1967). *Acta cryst.* **22**, 885–893.

MAIN, P., HULL, S. E., LESSINGER, L., GERMAIN, G., DECLERCQ, J.-P. & WOOLFSON, M. M. (1978). *MULTAN*78. *A System of Computer Programs for the Automatic Solution of Crystal Structures from X-ray Diffraction Data.* Univs. of York, England, and Louvain, Belgium.

SAKURAI, T. & KOBAYASHI, K. (1979). *Rikagaku Kenkyusho Hokoku*, **55**, 69–77.

VOOGD, J., VERZIJL, B. H. M. & DUISENBERG, A. J. M. (1980). *Acta Cryst.* B**36**, 2805–2806.

Acta Cryst. (1986). C**42**, 1881–1882

N,N'-Dimethyl-*N,N'*-ethylenebis(nicotinamide)

BY YVONNE A. ONATE, CRISTIAN O. FRANCO, JIAAN YANG, LI SHUI, GEORGE R. NEWKOME, FRANK R. FRONCZEK AND STEVEN F. WATKINS

Department of Chemistry, Louisiana State University, Baton Rouge, Louisiana 70803-1804, *USA*

(*Received* 22 *May* 1986; *accepted* 25 *June* 1986)

Abstract. $C_{16}H_{18}N_4O_2$, $M_r = 298{\cdot}4$, monoclinic, $P2_1/c$, $a = 8{\cdot}469$ (2), $b = 9{\cdot}727$ (3), $c = 9{\cdot}174$ (4) Å, $\beta = 92{\cdot}00$ (3)°, $V = 755{\cdot}3$ (8) Å^3, $Z = 2$, $D_x = 1{\cdot}312$ g cm^{-3}, Mo $K\alpha$, $\lambda = 0{\cdot}71073$ Å, $\mu = 0{\cdot}84$ cm^{-1}, $F(000) = 316$, $T = 297$ K, $R = 0{\cdot}041$ for 1391 observations (of 2193 unique data). The centrosymmetric molecule has a conformation in the crystal very similar to that observed in the phenyl analog, *N,N'*-dimethyl-*N,N'*-dibenzoylethylenediamine. The *N*-methyl group is oriented *syn* to the carboxyl group [O—C(3)—N(1)—C(2) torsion angle 2·4 (2)°], and the pyridine is twisted out of the carboxamide plane by 71·8 (2)° [torsion angle C(8)—C(4)—C(3)—O]. Pyridine C—C distances range from 1·368 (2) to 1·381 (1) Å, pyridine C—N lengths are 1·332 (2) and 1·338 (2) Å, and the central C—N bond of the amide linkage has length 1·342 (1) Å.

0108-2701/86/121881-02$01.50