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Guanidinium 2-carboxy-6-nitrobenzoate monohydrate: a two-dimensional hydrogen-bonded network structure

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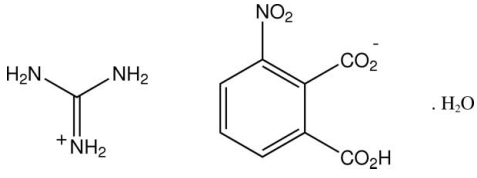
Key indicators: single-crystal X-ray study; T = 297 K; mean σ(C–C) = 0.003 Å; R factor = 0.047; wR factor = 0.147; data-to-parameter ratio = 13.2.

In the structure of the title compound, $CH_6N_3^+\cdot C_8H_4NO_6^-\cdot H_2O$, obtained from the reaction of guanidine carbonate with 3-nitrophthalic acid, the 2-carboxylic acid group is deprotonated and participates in an asymmetric cyclic $R_2^1(6)$ hydrogen-bonding association with the guanidine cation together with a bridging water molecule of solvation. A conjoint $R_1^2(7)$ facial association involving a nitro O-atom acceptor together with a further five guanidinium N—H···O hydrogen bonds, as well as a strong carboxyl–water O—H···O interaction [2.528 (3) Å], give a two-dimensional network structure.

Related literature

For related literature, see: Bernstein *et al.* (1995); Glidewell *et al.* (2003, 2005); Guo (2004); Smith *et al.* (2001, 2005); Smith, Wermuth & White (2007); Smith, Wermuth, Healy & White (2007).



Experimental

Crystal data

$CH_6N_3^+\cdot C_8H_4NO_6^-\cdot H_2O$
M_r = 288.23
Monoclinic, $P2_1/c$
a = 14.758 (3) Å
b = 12.5955 (19) Å
c = 6.8423 (12) Å
β = 100.006 (16)°
V = 1252.5 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.13 mm^{-1}
T = 297 (2) K
0.40 × 0.35 × 0.20 mm

Data collection

Rigaku AFC-7R diffractometer
Absorption correction: ψ scan (*TEXSAN for Windows*; Molecular Structure Corporation, 1999)
T_{min} = 0.949, T_{max} = 0.974
3307 measured reflections
2872 independent reflections
2080 reflections with $I > 2\sigma(I)$
R_{int} = 0.028
3 standard reflections
frequency: 150 min
intensity decay: 1.2%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.147
S = 0.86
2872 reflections
217 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1W···O21B	0.88 (5)	1.90 (5)	2.777 (3)	176 (3)
O1W—H2W···O21A^{i}	0.85 (5)	1.91 (5)	2.764 (3)	173 (4)
O11A—H11A···O1W^{ii}	0.89 (4)	1.65 (4)	2.528 (3)	169 (4)
N12—H12A···O21A^{iii}	0.91 (4)	2.06 (4)	2.946 (3)	167 (3)
N12—H12B···O21B	0.85 (4)	2.58 (4)	3.286 (3)	141 (3)
N12—H12B···O31A	0.85 (4)	2.51 (3)	2.964 (3)	114 (3)
N22—H22A···O11B^{iv}	0.91 (4)	1.96 (4)	2.846 (3)	162 (3)
N22—H22B···O21B^{v}	0.87 (4)	2.54 (3)	3.183 (3)	132 (3)
N32—H32A···O21B	0.83 (3)	2.11 (3)	2.905 (3)	162 (3)
N32—H32B···O11B^{iv}	0.85 (4)	2.51 (4)	3.152 (3)	134 (3)
N32—H32B···O21A^{iv}	0.85 (4)	2.30 (4)	3.048 (3)	148 (3)

Symmetry codes: (i) $x, y, z+1$; (ii) $x, -y+\frac{5}{2}, z-\frac{1}{2}$; (iii) $x, -y+\frac{3}{2}, z+\frac{1}{2}$; (iv) $-x, -y+2, -z+1$; (v) $-x, y-\frac{1}{2}, -z+\frac{3}{2}$.

Data collection: *MSC/AFC Diffractometer Control Software* (Molecular Structure Corporation, 1999); cell refinement: *MSC/AFC Diffractometer Control Software*; data reduction: *TEXSAN for Windows* (Molecular Structure Corporation, 1999); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *PLATON*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WN2170).

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supplementary materials

Acta Cryst. (2007). E**63**, o3527-o3528 [**doi:10.1107/S1600536807034356**]

Guanidinium 2-carboxy-6-nitrobenzoate monohydrate: a two-dimensional hydrogen-bonded network structure

G. Smith, U. D. Wermuth and P. C. Healy

Comment

The structures of the guanidinium salts of nitro-substituted benzoic acids are not numerous in the crystallographic literature. Among these are the 1:1 anhydrous guanidinium salts of 3,5-dinitrosalicylic acid (Smith *et al.*, 2001), 3,5-dinitrobenzoic acid (Smith, Wermuth & White, 2007) and 4-nitroanthranilic acid (a monohydrate) (Smith *et al.*, 2007). The nitro-substituted aromatic dicarboxylic acids provide additional potential for structure extension and some structures of 1:1 Lewis base salts of these acids are known, *e.g.* the anhydrous compounds of 3-nitrophthalic acid with 3-iodoaniline (Glidewell *et al.*. 2005) and 4-iodoaniline (Glidewell *et al.*. 2003 and the dihydrate with brucine (Smith *et al.*, 2005). In the 1:1 dihydrate salt with piperazine (Guo, 2004), the phthalate species is dianionic.

Our 1:1 stoichiometric reaction of 3-nitrophthalic acid with guanidinium carbonate in methanol surprisingly gave good crystals of a hydrated salt guanidinium 2-carboxy-6-nitrobenzoate monohydrate, $CH_6N_3^+\cdot C_8H_4NO_6^-\cdot H_2O$, which is reported here. In the title compound, the usual proton transfer occurs from the central (C2) carboxylic acid group which is then involved in a direct hydrogen-bonding interaction with a guanidinium proton (Fig. 1). The guanidinium protons are involved in eight hydrogen bonds with all but one of the available O acceptors (nitro O31B) (Table 1). These include the water molecule of solvation which also provides a bridging link between the two separate carboxylate O-acceptors ($O21A^{i}$, O21B: symmetry code (i), $x, y, z + 1$], extending the structure down the *c* cell direction. With the guanidinium cation there is an asymmetric cyclic $R_2^1(6)$ (Bernstein *et al.*, 1995) interaction also with a carboxylate O-acceptor together with a conjoint $R_1^2(7)$ nitro-O interaction. The carboxylic acid proton gives a strong hydrogen bond with the water molecule [O···O, 2.528 (2) Å], the overall result being a two-dimensional network structure (Fig. 2).

Within the 3-nitrophthalate anion, the carboxylate group is close to perpendicular to the plane of the benzene ring [C1—C2—C21—O21A, 101.2 (2)°], while the carboxylic acid group is close to coplanar [C2—C1—C11—O11A, 173.34 (19)°]. The nitro group is intermediate between these [C2—3—N31—O31B, 151.2 (2) °]. This conformation is similar to that found in other acid salts of 3-nitrophthalic acid (Smith *et al.*, 2005; Glidewell *et al.* 2003, 2005). In addition there is an intramolecular aromatic ring hydrogen bond [C6–H···O11A: 2.706 (3) Å] associated with the carboxylic acid group.

Experimental

The title compound was synthesized by heating together 1 mmol quantities of 3-nitrophthalic acid and guanidine carbonate in 50 ml of methanol under reflux for 10 minutes. After concentration to *ca* 30 ml, partial room temperature evaporation of the hot-filtered solution gave colourless crystal prisms (m.p. 395–396 K).

Refinement

Hydrogen atoms involved in hydrogen-bonding interactions were located by difference methods and their positional and isotropic displacement parameters were refined. The ranges of refined bond lengths were N—H = 0.83 (3)–0.91 (4) Å and O—H = 0.85 (5)–0.89 (4) Å. The aromatic H atoms were included in the refinement in calculated positions (C—H = 0.95 Å) using a riding model approximation, with U_{iso}(H) = 1.2U_{eq}(C).

Figures

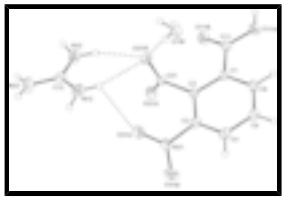


Fig. 1. Molecular configuration and atom naming scheme for the guanidinium cation, the 3-nitrophthalate anion and the water molecule of solvation in the title compound. Displacement ellipsoids are drawn at the 40% probability level. Dashed lines indicate hydrogen bonds.

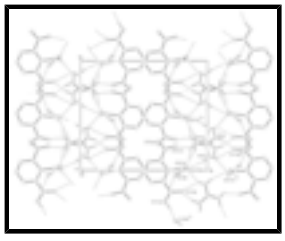


Fig. 2. The hydrogen-bonded framework structure of the title compound, viewed down the *c* axial direction, showing hydrogen-bonding associations as dashed lines. For symmetry codes, see Table 1.

guanidinium 2-carboxy-6-nitrobenzoate monohydrate

Crystal data

$CH_6N_3^+ \cdot C_8H_4NO_6^- \cdot H_2O$	F_{000} = 600
M_r = 288.23	D_x = 1.528 Mg m^{-3}
Monoclinic, $P2_1/c$	Melting point: 395-396 K
Hall symbol: -P 2ybc	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 14.758 (3) Å	Cell parameters from 25 reflections
b = 12.5955 (19) Å	θ = 12.6–17.5º
c = 6.8423 (12) Å	μ = 0.13 mm^{-1}
β = 100.006 (16)º	T = 297 (2) K
V = 1252.5 (4) Å^3	Cut block, colourless
Z = 4	0.40 × 0.35 × 0.20 mm

Data collection

Rigaku AFC-7R diffractometer	R_{int} = 0.028
Radiation source: rotating anode	θ_{max} = 27.5º
Monochromator: graphite	θ_{min} = 2.8º
T = 297(2) K	h = −18→19

ω/2θ scans	$k = 0 \rightarrow 16$
Absorption correction: ψ scan (TEXSAN for Windows; Molecular Structure Corporation, 1999)	$l = -8 \rightarrow 3$
$T_{min} = 0.949$, $T_{max} = 0.974$	3 standard reflections
3307 measured reflections	every 150 min
2872 independent reflections	intensity decay: 1.2%
2080 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.047$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.147$	$w = 1/[\sigma^2(F_o^2) + (0.1P)^2 + 5.5554P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.86$	$(\Delta/\sigma)_{max} = 0.001$
2872 reflections	$\Delta\rho_{max} = 0.33$ e Å^{-3}
217 parameters	$\Delta\rho_{min} = -0.40$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O11A	0.33502 (12)	1.28306 (13)	0.6829 (3)	0.0402 (6)
O11B	0.21101 (11)	1.19235 (14)	0.5452 (3)	0.0436 (6)
O21A	0.16688 (11)	0.96584 (13)	0.4120 (2)	0.0331 (5)
O21B	0.16155 (10)	0.98708 (14)	0.7330 (2)	0.0339 (5)
O31A	0.25485 (12)	0.78120 (15)	0.6336 (3)	0.0480 (6)
O31B	0.38515 (13)	0.73913 (16)	0.5523 (3)	0.0551 (7)
N31	0.33335 (13)	0.80279 (15)	0.6115 (3)	0.0338 (6)
C1	0.34791 (14)	1.09732 (17)	0.6688 (3)	0.0266 (6)
C2	0.30745 (13)	0.99645 (16)	0.6370 (3)	0.0240 (5)
C3	0.36807 (14)	0.91080 (17)	0.6560 (3)	0.0270 (6)

C4	0.46275 (15)	0.92106 (19)	0.7140 (4)	0.0337 (7)
C5	0.50006 (15)	1.0204 (2)	0.7553 (4)	0.0374 (7)
C6	0.44276 (15)	1.10785 (19)	0.7288 (4)	0.0346 (7)
C11	0.29065 (15)	1.19500 (17)	0.6278 (3)	0.0283 (6)
C21	0.20296 (13)	0.98198 (16)	0.5881 (3)	0.0250 (6)
N12	0.08940 (15)	0.7473 (2)	0.8170 (3)	0.0406 (7)
N22	−0.05841 (16)	0.6993 (2)	0.6799 (4)	0.0454 (7)
N32	−0.01159 (16)	0.87191 (19)	0.6668 (4)	0.0409 (7)
C12	0.00621 (15)	0.77276 (19)	0.7218 (3)	0.0313 (6)
O1W	0.25121 (17)	1.04247 (17)	1.1102 (4)	0.0536 (7)
H4	0.50130	0.86020	0.72510	0.0400*
H5	0.56420	1.02870	0.80120	0.0450*
H6	0.46850	1.17680	0.75190	0.0420*
H11A	0.299 (3)	1.340 (3)	0.655 (5)	0.069 (11)*
H12A	0.104 (2)	0.678 (3)	0.838 (5)	0.055 (9)*
H12B	0.130 (2)	0.796 (3)	0.839 (5)	0.056 (10)*
H22A	−0.113 (3)	0.720 (3)	0.605 (6)	0.071 (11)*
H22B	−0.050 (2)	0.637 (3)	0.733 (5)	0.056 (9)*
H32A	0.030 (2)	0.917 (3)	0.683 (5)	0.058 (10)*
H32B	−0.066 (3)	0.894 (3)	0.629 (5)	0.063 (10)*
H1W	0.222 (3)	1.022 (3)	0.994 (7)	0.071 (12)*
H2W	0.221 (3)	1.018 (3)	1.196 (7)	0.078 (13)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O11A	0.0312 (9)	0.0252 (8)	0.0599 (12)	0.0003 (7)	−0.0037 (8)	−0.0040 (8)
O11B	0.0257 (8)	0.0321 (9)	0.0679 (12)	0.0020 (7)	−0.0064 (8)	0.0011 (8)
O21A	0.0271 (8)	0.0384 (9)	0.0304 (8)	−0.0047 (7)	−0.0042 (6)	−0.0010 (7)
O21B	0.0254 (8)	0.0420 (9)	0.0352 (9)	−0.0050 (7)	0.0077 (6)	−0.0025 (7)
O31A	0.0332 (9)	0.0341 (9)	0.0750 (14)	−0.0063 (7)	0.0045 (9)	−0.0017 (9)
O31B	0.0406 (10)	0.0408 (10)	0.0789 (15)	0.0122 (8)	−0.0036 (10)	−0.0200 (10)
N31	0.0288 (9)	0.0273 (9)	0.0407 (11)	0.0034 (8)	−0.0069 (8)	−0.0018 (8)
C1	0.0206 (9)	0.0274 (10)	0.0309 (11)	0.0001 (8)	0.0019 (8)	0.0003 (8)
C2	0.0200 (9)	0.0279 (10)	0.0232 (9)	−0.0004 (7)	0.0015 (7)	−0.0008 (8)
C3	0.0232 (10)	0.0267 (10)	0.0294 (10)	0.0007 (8)	−0.0004 (8)	−0.0009 (8)
C4	0.0218 (10)	0.0343 (12)	0.0427 (13)	0.0058 (9)	−0.0008 (9)	0.0025 (10)
C5	0.0187 (9)	0.0401 (13)	0.0510 (14)	0.0000 (9)	−0.0008 (9)	0.0020 (11)
C6	0.0246 (10)	0.0307 (11)	0.0462 (13)	−0.0047 (9)	−0.0004 (9)	0.0000 (10)
C11	0.0269 (10)	0.0262 (10)	0.0316 (11)	−0.0008 (8)	0.0045 (8)	−0.0002 (8)
C21	0.0200 (9)	0.0217 (9)	0.0321 (11)	0.0003 (7)	0.0011 (8)	0.0004 (8)
N12	0.0273 (10)	0.0456 (13)	0.0464 (12)	0.0044 (10)	−0.0008 (9)	0.0084 (10)
N22	0.0350 (11)	0.0429 (13)	0.0551 (14)	−0.0070 (10)	−0.0011 (10)	0.0137 (11)
N32	0.0274 (10)	0.0376 (12)	0.0559 (14)	0.0050 (9)	0.0026 (9)	0.0080 (10)
C12	0.0251 (10)	0.0376 (12)	0.0312 (11)	0.0023 (9)	0.0047 (8)	0.0055 (9)
O1W	0.0732 (15)	0.0483 (12)	0.0396 (11)	−0.0297 (11)	0.0107 (11)	−0.0049 (9)

Geometric parameters (Å, °)

O11A—C11	1.310 (3)	N22—H22B	0.87 (4)
O11B—C11	1.213 (3)	N22—H22A	0.91 (4)
O21A—C21	1.247 (2)	N32—H32B	0.85 (4)
O21B—C21	1.253 (2)	N32—H32A	0.83 (3)
O31A—N31	1.225 (3)	C1—C6	1.395 (3)
O31B—N31	1.224 (3)	C1—C11	1.491 (3)
O11A—H11A	0.89 (4)	C1—C2	1.405 (3)
O1W—H1W	0.88 (5)	C2—C3	1.393 (3)
O1W—H2W	0.85 (5)	C2—C21	1.531 (3)
N31—C3	1.467 (3)	C3—C4	1.391 (3)
N12—C12	1.325 (3)	C4—C5	1.376 (3)
N22—C12	1.324 (3)	C5—C6	1.381 (3)
N32—C12	1.318 (3)	C4—H4	0.9500
N12—H12B	0.85 (4)	C5—H5	0.9500
N12—H12A	0.91 (4)	C6—H6	0.9500
C11—O11A—H11A	112 (3)	N31—C3—C4	116.29 (19)
H1W—O1W—H2W	107 (4)	N31—C3—C2	120.22 (18)
O31A—N31—C3	118.95 (19)	C3—C4—C5	119.3 (2)
O31A—N31—O31B	123.6 (2)	C4—C5—C6	119.0 (2)
O31B—N31—C3	117.41 (19)	C1—C6—C5	121.5 (2)
C12—N12—H12B	118 (2)	O11A—C11—O11B	123.6 (2)
C12—N12—H12A	119 (2)	O11A—C11—C1	113.95 (19)
H12A—N12—H12B	122 (3)	O11B—C11—C1	122.4 (2)
H22A—N22—H22B	123 (3)	O21A—C21—C2	118.40 (18)
C12—N22—H22A	117 (2)	O21B—C21—C2	115.60 (17)
C12—N22—H22B	120 (2)	O21A—C21—O21B	126.01 (19)
H32A—N32—H32B	117 (3)	C3—C4—H4	120.00
C12—N32—H32B	122 (3)	C5—C4—H4	120.00
C12—N32—H32A	120 (2)	C6—C5—H5	121.00
C2—C1—C6	120.6 (2)	C4—C5—H5	121.00
C6—C1—C11	118.9 (2)	C5—C6—H6	119.00
C2—C1—C11	120.35 (19)	C1—C6—H6	119.00
C3—C2—C21	122.30 (18)	N12—C12—N22	120.6 (2)
C1—C2—C3	115.93 (18)	N12—C12—N32	119.4 (2)
C1—C2—C21	121.77 (18)	N22—C12—N32	120.0 (2)
C2—C3—C4	123.5 (2)		
O31A—N31—C3—C2	−28.2 (3)	C6—C1—C11—O11B	167.8 (2)
O31A—N31—C3—C4	152.5 (2)	C1—C2—C3—N31	−175.49 (18)
O31B—N31—C3—C2	151.2 (2)	C1—C2—C3—C4	3.7 (3)
O31B—N31—C3—C4	−28.0 (3)	C21—C2—C3—N31	5.6 (3)
C6—C1—C2—C3	−4.2 (3)	C21—C2—C3—C4	−175.3 (2)
C6—C1—C2—C21	174.8 (2)	C1—C2—C21—O21A	101.2 (2)
C11—C1—C2—C3	172.36 (18)	C1—C2—C21—O21B	−79.2 (3)
C11—C1—C2—C21	−8.7 (3)	C3—C2—C21—O21A	−79.9 (3)
C2—C1—C6—C5	1.2 (4)	C3—C2—C21—O21B	99.7 (2)
C11—C1—C6—C5	−175.4 (2)	N31—C3—C4—C5	179.1 (2)

C2—C1—C11—O11A	173.34 (19)	C2—C3—C4—C5	−0.1 (4)
C2—C1—C11—O11B	−8.8 (3)	C3—C4—C5—C6	−3.1 (4)
C6—C1—C11—O11A	−10.1 (3)	C4—C5—C6—C1	2.5 (4)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1W—H1W···O21B	0.88 (5)	1.90 (5)	2.777 (3)	176 (3)
O1W—H2W···O21A^{i}	0.85 (5)	1.91 (5)	2.764 (3)	173 (4)
O11A—H11A···O1W^{ii}	0.89 (4)	1.65 (4)	2.528 (3)	169 (4)
N12—H12A···O21A^{iii}	0.91 (4)	2.06 (4)	2.946 (3)	167 (3)
N12—H12B···O21B	0.85 (4)	2.58 (4)	3.286 (3)	141 (3)
N12—H12B···O31A	0.85 (4)	2.51 (3)	2.964 (3)	114 (3)
N22—H22A···O11B^{iv}	0.91 (4)	1.96 (4)	2.846 (3)	162 (3)
N22—H22B···O21B^{v}	0.87 (4)	2.54 (3)	3.183 (3)	132 (3)
N32—H32A···O21B	0.83 (3)	2.11 (3)	2.905 (3)	162 (3)
N32—H32B···O11B^{iv}	0.85 (4)	2.51 (4)	3.152 (3)	134 (3)
N32—H32B···O21A^{iv}	0.85 (4)	2.30 (4)	3.048 (3)	148 (3)
C4—H4···O11A^{vi}	0.9500	2.5800	3.420 (3)	148.00
C6—H6···O11A	0.9500	2.3600	2.706 (3)	101.00
C6—H6···O31B^{vii}	0.9500	2.4600	3.179 (3)	132.00

Symmetry codes: (i) *x*, *y*, *z*+1; (ii) *x*, −*y*+5/2, *z*−1/2; (iii) *x*, −*y*+3/2, *z*+1/2; (iv) −*x*, −*y*+2, −*z*+1; (v) −*x*, *y*−1/2, −*z*+3/2; (vi) −*x*+1, *y*−1/2, −*z*+3/2; (vii) −*x*+1, *y*+1/2, −*z*+3/2.

Fig. 1

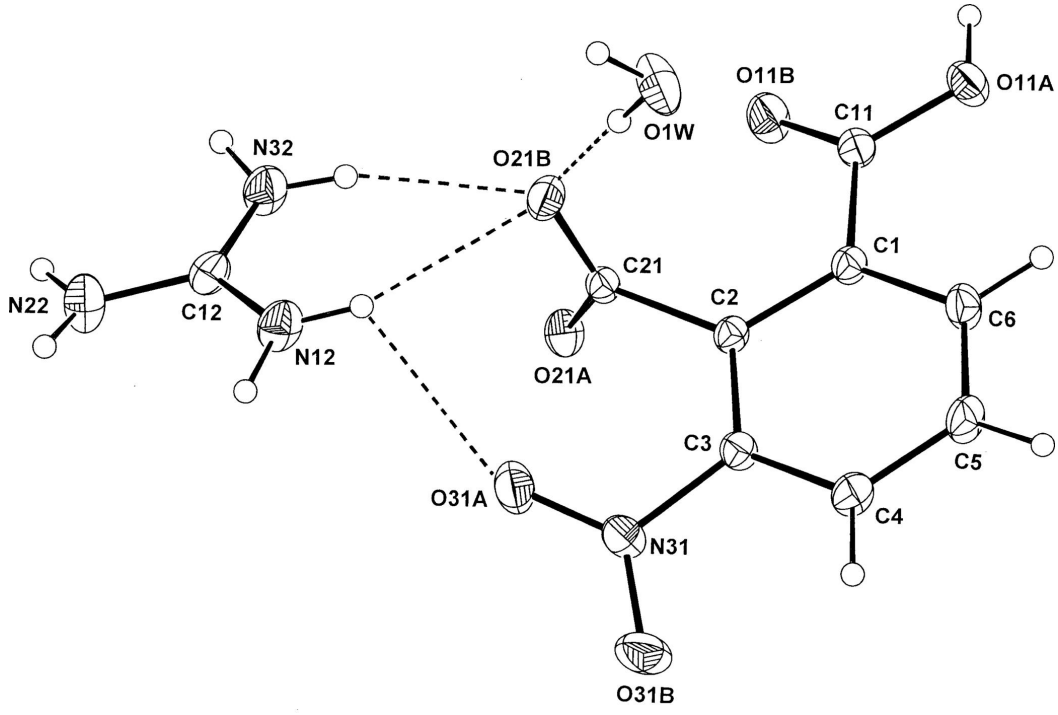
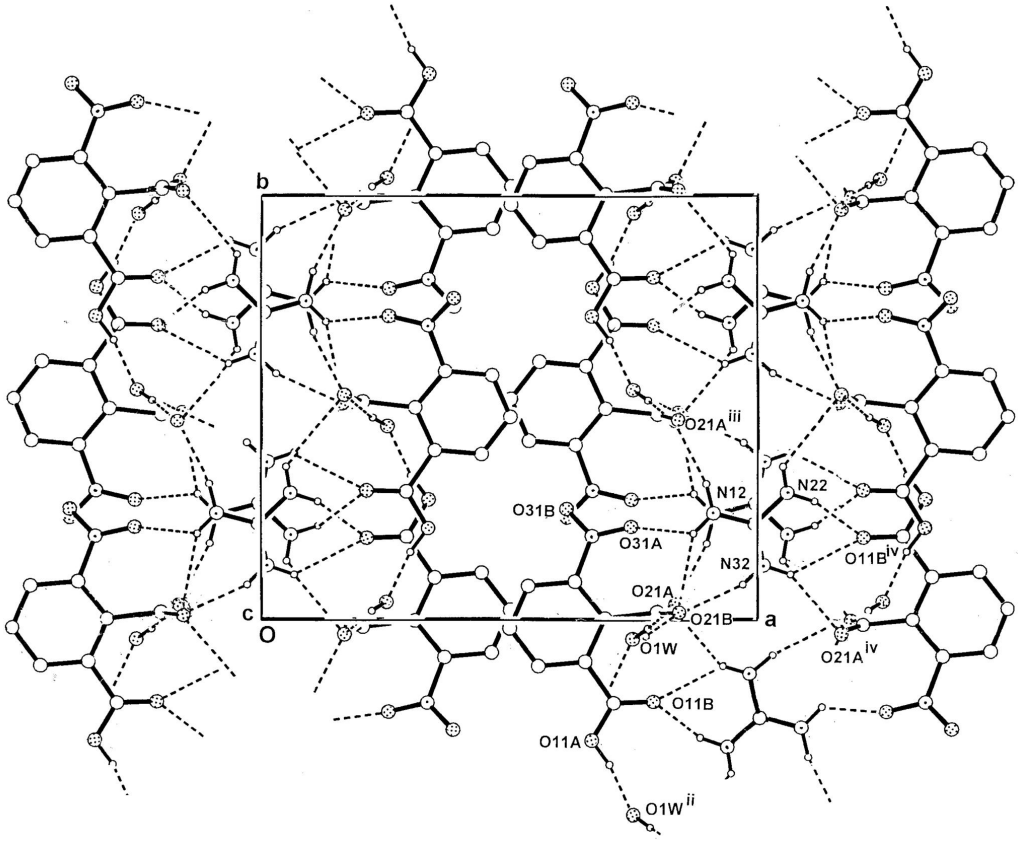

O11B
O11A
C11
O1W
N32
O21B
C1
C21
N22
C12
C2
C6
N12
O21A
C3
C5
O31A
C4
N31
O31B

Fig. 2


b
c
O
a
O21A iii
N12
N22
O31B
O31A
O11B iv
N32
O21A
O21B
O1W
O21A iv
O11B
O11A
O1W ii