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Bis(2-methylimidazolium) terephthalate bis(2-methylimidazole) tetrahydrate

Shao-hua Qu

Department of Physics, Xiangfan University, Hubei 441053, People's Republic of China
Correspondence e-mail: shaohua_qu@126.com

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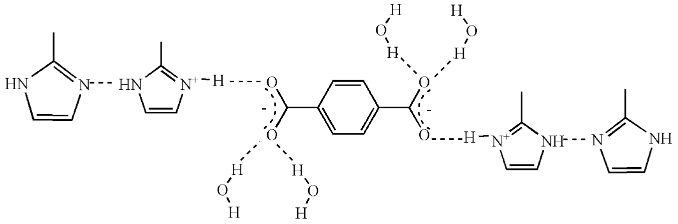
Key indicators: single-crystal X-ray study; *T* = 297 K; mean σ(C–C) = 0.002 Å; *R* factor = 0.046; *wR* factor = 0.151; data-to-parameter ratio = 15.5.

The title compound, $2C_4H_7N_2^+\cdot C_8H_4O_4^{2-}\cdot 2C_4H_6N_2\cdot 4H_2O$, was formed by the reaction of terephthalic acid (H_2tere) and 2-methylimidazole (2-MeIm). The asymmetric unit consists of half a tere dianion, a 2-methylimidazolium cation, a neutral 2-MeIm molecule and two solvent water molecules, the formula unit being generated by crystallographic inversion symmetry. A combination of N—H⋯N, N—H⋯O, O—H⋯O and C—H⋯O hydrogen bonds, C—H⋯π interactions, and π–π interactions [with centroid–centroid distances of 3.654 (1) and 3.337 (1) Å] link the independent components into a three-dimensional network.

Related literature

For related literature, see: Yang & Qu (2006*a*,*b*); Bernstein *et al.* (1995).



Experimental

Crystal data

$2C_4H_7N_2^+\cdot C_8H_4O_4^{2-}\cdot$-
$2C_4H_6N_2\cdot 4H_2O$
M_r = 566.62
Triclinic, $P\overline{1}$
a = 6.8753 (4) Å
b = 10.5598 (7) Å
c = 11.2757 (7) Å
α = 71.105 (1)°
β = 78.984 (1)°
γ = 74.738 (1)°
V = 742.17 (8) Å^3
Z = 1
Mo *Kα* radiation
μ = 0.10 mm^{-1}
T = 297 (2) K
0.40 × 0.23 × 0.20 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1997)
T_{min} = 0.956, T_{max} = 0.981
8374 measured reflections
3175 independent reflections
2301 reflections with $I > 2\sigma(I)$
R_{int} = 0.051

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.151
S = 1.10
3175 reflections
205 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

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

Cg is the centroid of the benzene ring.

D—H⋯*A*	*D*—H	H⋯*A*	*D*⋯*A*	*D*—H⋯*A*
N1—H1*A*⋯N3	0.882 (9)	1.830 (10)	2.7078 (18)	173.5 (17)
N2—H2*A*⋯O2	0.92 (2)	1.78 (2)	2.6965 (17)	175.6 (17)
O3—H3*B*⋯O1	0.74 (3)	2.08 (3)	2.8138 (18)	170 (3)
O4—H4*B*⋯O1	0.90 (3)	1.87 (3)	2.7723 (17)	175 (2)
O3—H3*A*⋯O2^{i}	0.87 (3)	1.94 (3)	2.812 (2)	176 (3)
O4—H4*A*⋯O3^{ii}	0.81 (3)	1.97 (3)	2.766 (2)	166 (3)
N4—H4*C*⋯O4^{iii}	0.85 (2)	1.94 (2)	2.7872 (19)	175.7 (18)
C12—H12*B*⋯O3^{iv}	0.96	2.59	3.542 (2)	169
C10—H10⋯*Cg*^{v}	0.93	2.89	3.700 (2)	147

Symmetry codes: (i) $x+1, y, z$; (ii) $-x+1, -y, -z$; (iii) $-x, -y+1, -z-1$; (iv) $x-1, y+1, z-1$; (v) $x, y, z-1$.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); 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: LH2502).

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supplementary materials

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Bis(2-methylimidazolium) terephthalate bis(2-methylimidazole) tetrahydrate

S. Qu

Comment

As part of our continuing studies involving H-bonding, C–H···π and π–π interactions in organic adducts (Yang and Qu, 2006*a*,2006*b*), we report here the molecular and supramolecular structure of an organic analog formed by terephthalic acid acid (tere) and 2-Methylimidazole (2-MeIm), namely Bis(2-Methylimidazolium) terephthalate bis(2-Methylimidazole) tetrahydrate.

In the title compound, the formula unit is composed of a tere dianion which lies on a crystallographic centre of inversion, two 2-MeIm cations, two neutral 2-MeIm molecules and four water solvent molecules (Fig.1). As expected, in the molecular structure both the carboxyl H atoms are transferred to the adjacent imine N atoms. The four incorporated water solvent molecules may help stabilize the crystal structure. However, the reason of the incorporation of another two neutral 2-MeIm molecules whether incidental or inevitable might be confirmed by modulating the reactant molar ration of tere *versus* 2-MeIm. The further research work is being undertaken.

The supramolecular structure is formed by a combination of N–H···N, N–H···O, O–H···O, C–H···O hydrogen bonds, C–H···π and π–π interactions which can be analysed in terms of several simple substructures.

Firstly, a combination of H-bonding formed between the tere dianions and two water molecules links the three independent components into a two-dimensional network running parallel to the (010) direction which is built from alternating $R^6_4(16)$ and $R^4_4(12)$ H-bonding rings (Fig.2) (Bernstein *et al.*, 1995). Secondly, the combination of N2–H2A···O2, N1–H1A···N3, N4–H4C···O4^{iii} and C12–H12B···O3^{iv} hydrogen bonds [symmetry codes as in Table 1] running along the [01–2] direction (Table 1) links the adjacent networks into a three-dimensional network. Finally, the crystal structure is consolidated by C–H···π [H···*Cg* = 2.89 Å, C–H···*Cg* (*x*,*y*,-1 + *z* and −*z*,-*y*,-*z*) = 147°, where *Cg* is the centroid of the benzene ring] and π–π interactions [*Cg*1–*Cg*1 (−1 − *x*,1 − *y*,-1 − *z*) centroid-centroid distance of 3.64 (1) and perpendicular distance of 3.34 Å; where *Cg*1 is the centroid of ring atoms N3/C9/N4/C/11/C10].

Experimental

All reagents and solvents were used as obtained without further purification. 2:1 molar amount of 2-methylimidazole (0.4 mmol, 32 mg) and terephthalic acid (0.2 mmol, 33 mg) were dissolved in 95% methanol (10 ml). The mixture was stirred for ten minutes at ambient temperature. The resulting colorless solution was kept in air for several days. Crystals suitable for single-crystal X-ray diffraction analysis were grown by slow evaporation of the solution at the bottom of the vessel.

Refinement

H atoms bonded to carbon atoms were located at the geometrical positions with C—H = 0.93 Å (aromatic) and 0.96 Å(methyl), and U_{iso}(H) = 1.2U_{eq}(aromatic C) and 1.5U_{eq}(methyl C). H atoms bonded to N and water O atoms were located from the difference maps with the N(or O)–H distances refined freely and their U_{iso} values being set 1.2 and 1.5 times of their carrier atoms for N and O atoms, respectively.

Figures

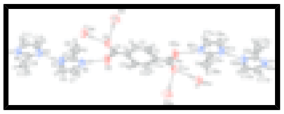

Fig. 1. Molecular structure showing the atom-numbering scheme·Displacement ellipsoids are drawn at the 50% probability level. Hydrogen bonds are shown as dashed lines. Atoms marked with 'a' are realted by the symmetry operator ($-x$, $-y$, $1 - z$).

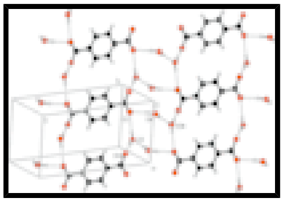

Fig. 2. Part of the crystal structure, showing the formation of the two-dimensional (010) network by hydrogen bonds formed between tere dianions and water molecules. Hydrogen bonds are shown as dashed lines. Atom marked with sign '#' and '$' are at symmetry positions ($1 + x,y,z$) and ($1 - x,-y,-z$), respectively.

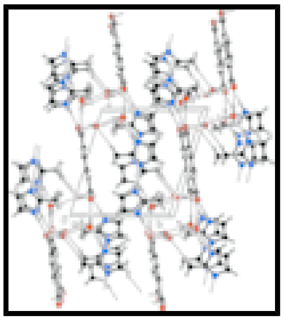

Fig. 3. Part of the crystal structure, showing the formation of the three-dimensional netwok by N2–H2A···O2, N1–H1A···N3, N4–H4C···O4^{iii} and C12–H12B···O3^{iv} hydrogen bonds. Hydrogen bonds are shown as dashed lines. Symmetry codes as in Table 1.

Bis(2-methylimidazolium) terephthalate bis(2-methylimidazole) tetrahydrate

Crystal data

$2C_4H_7N_2^+\cdot C_8H_4O_4^{2-}\cdot 2C_4H_6N_2\cdot 4H_2O$	$Z = 1$
$M_r = 566.62$	$F_{000} = 302$
Triclinic, $P\bar{1}$	$D_x = 1.268$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 6.8753$ (4) Å	Cell parameters from 3333 reflections
$b = 10.5598$ (7) Å	$\theta = 2.4$–27.2°
$c = 11.2757$ (7) Å	$\mu = 0.10$ mm^{-1}
$\alpha = 71.105$ (1)°	$T = 297$ (2) K
$\beta = 78.984$ (1)°	Block, colorless
$\gamma = 74.738$ (1)°	0.40 × 0.23 × 0.20 mm
$V = 742.17$ (8) Å^3	

Data collection

Bruker SMART APEX CCD area-detector diffractometer	3175 independent reflections
Radiation source: fine focus sealed Siemens Mo tube	2301 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.051$

T = 297(2) K
0.3° wide ω exposures scans
Absorption correction: multi-scan (SADABS; Sheldrick, 1997)
$T_{\min}$ = 0.956, $T_{\max}$ = 0.981
8374 measured reflections

$\theta_{\max}$ = 27.0º
$\theta_{\min}$ = 1.9º
$h = -8 \rightarrow 8$
$k = -13 \rightarrow 13$
$l = -14 \rightarrow 14$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.046$
$wR(F^2) = 0.151$
S = 1.10
3175 reflections
205 parameters
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0879P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.002$
$\Delta\rho_{\max}$ = 0.22 e Å^{-3}
$\Delta\rho_{\min}$ = −0.20 e Å^{-3}
Extinction correction: SHELXL97, $\mathrm{Fc}^*=\mathrm{kFc}[1+0.001\mathrm{xFc}^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.091 (12)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

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 $F^2 > 2\mathrm{sigma}(F^2)$ 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}
C1	0.0079 (2)	0.06134 (12)	0.36920 (12)	0.0394 (3)
C2	0.1787 (2)	0.03001 (14)	0.43034 (13)	0.0464 (4)
H2	0.2997	0.0501	0.3841	0.056*
C3	0.1712 (2)	−0.03109 (14)	0.55977 (13)	0.0467 (4)
H3	0.2874	−0.0520	0.5992	0.056*
C4	0.0135 (2)	0.13144 (13)	0.22876 (12)	0.0444 (4)
O1	0.17895 (18)	0.15475 (12)	0.16824 (9)	0.0610 (3)
O2	−0.15041 (18)	0.16592 (12)	0.18190 (10)	0.0645 (4)
O3	0.5850 (2)	0.00820 (15)	0.17111 (15)	0.0791 (4)

H3A	0.662 (4)	0.061 (3)	0.175 (3)	0.119*
H3B	0.484 (4)	0.055 (3)	0.169 (3)	0.119*
C5	−0.2141 (2)	0.33062 (15)	−0.14696 (13)	0.0494 (4)
C6	−0.2641 (3)	0.55302 (18)	−0.18719 (17)	0.0655 (5)
H6	−0.2866	0.6460	−0.2304	0.079*
C7	−0.2412 (3)	0.49718 (18)	−0.06486 (16)	0.0659 (5)
H7	−0.2456	0.5439	−0.0069	0.079*
C8	−0.1840 (3)	0.19192 (17)	−0.16068 (17)	0.0678 (5)
H8A	−0.0457	0.1625	−0.1934	0.102*
H8B	−0.2729	0.1941	−0.2177	0.102*
H8C	−0.2139	0.1291	−0.0798	0.102*
N1	−0.2483 (2)	0.44791 (13)	−0.23739 (12)	0.0556 (4)
H1A	−0.256 (3)	0.4523 (18)	−0.3158 (10)	0.067*
N2	−0.2101 (2)	0.35862 (15)	−0.04107 (12)	0.0565 (4)
H2A	−0.190 (3)	0.290 (2)	0.0328 (19)	0.068*
N3	−0.2465 (2)	0.47035 (12)	−0.48371 (11)	0.0518 (4)
N4	−0.2631 (2)	0.56086 (15)	−0.68589 (12)	0.0561 (4)
H4C	−0.277 (3)	0.6260 (19)	−0.7539 (19)	0.067*
C9	−0.2679 (2)	0.58589 (15)	−0.57583 (14)	0.0489 (4)
C10	−0.2261 (3)	0.36807 (16)	−0.53889 (16)	0.0590 (4)
H10	−0.2077	0.2750	−0.4964	0.071*
C11	−0.2366 (3)	0.42301 (17)	−0.66313 (16)	0.0627 (5)
H11	−0.2277	0.3764	−0.7219	0.075*
C12	−0.2916 (3)	0.72429 (17)	−0.56221 (17)	0.0671 (5)
H12A	−0.3974	0.7377	−0.4954	0.101*
H12B	−0.3263	0.7924	−0.6398	0.101*
H12C	−0.1664	0.7324	−0.5425	0.101*
O4	0.2874 (2)	0.22477 (14)	−0.09066 (13)	0.0788 (4)
H4A	0.318 (4)	0.149 (3)	−0.102 (2)	0.118*
H4B	0.246 (4)	0.207 (3)	−0.007 (3)	0.118*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0524 (8)	0.0337 (6)	0.0306 (7)	−0.0078 (5)	−0.0061 (6)	−0.0079 (5)
C2	0.0505 (8)	0.0529 (8)	0.0344 (7)	−0.0156 (6)	−0.0022 (6)	−0.0088 (6)
C3	0.0518 (9)	0.0516 (8)	0.0351 (7)	−0.0111 (6)	−0.0116 (6)	−0.0066 (6)
C4	0.0591 (9)	0.0395 (7)	0.0329 (7)	−0.0088 (6)	−0.0060 (7)	−0.0092 (6)
O1	0.0697 (8)	0.0692 (7)	0.0340 (6)	−0.0158 (6)	−0.0017 (5)	−0.0032 (5)
O2	0.0730 (8)	0.0773 (8)	0.0369 (6)	−0.0174 (6)	−0.0187 (5)	0.0000 (5)
O3	0.0703 (9)	0.0749 (9)	0.0892 (10)	−0.0070 (7)	−0.0135 (8)	−0.0244 (8)
C5	0.0502 (8)	0.0547 (9)	0.0383 (8)	−0.0104 (6)	−0.0063 (6)	−0.0069 (7)
C6	0.0890 (13)	0.0511 (9)	0.0538 (10)	−0.0136 (8)	−0.0155 (9)	−0.0086 (7)
C7	0.0809 (12)	0.0653 (11)	0.0543 (10)	−0.0108 (9)	−0.0133 (9)	−0.0218 (8)
C8	0.0811 (12)	0.0575 (10)	0.0608 (11)	−0.0162 (8)	−0.0069 (9)	−0.0118 (8)
N1	0.0727 (9)	0.0548 (8)	0.0370 (7)	−0.0150 (6)	−0.0130 (6)	−0.0055 (6)
N2	0.0633 (8)	0.0624 (8)	0.0367 (7)	−0.0072 (6)	−0.0109 (6)	−0.0067 (6)
N3	0.0634 (8)	0.0480 (7)	0.0406 (7)	−0.0113 (6)	−0.0102 (6)	−0.0065 (5)

N4	0.0655 (9)	0.0598 (8)	0.0358 (7)	−0.0082 (6)	−0.0057 (6)	−0.0086 (6)
C9	0.0510 (8)	0.0514 (8)	0.0411 (8)	−0.0114 (6)	−0.0064 (6)	−0.0083 (7)
C10	0.0722 (11)	0.0473 (9)	0.0551 (10)	−0.0091 (7)	−0.0091 (8)	−0.0136 (7)
C11	0.0756 (11)	0.0620 (10)	0.0517 (9)	−0.0064 (8)	−0.0069 (8)	−0.0250 (8)
C12	0.0872 (12)	0.0518 (9)	0.0613 (11)	−0.0180 (8)	−0.0138 (9)	−0.0096 (8)
O4	0.1040 (11)	0.0723 (9)	0.0391 (7)	−0.0065 (7)	−0.0004 (7)	−0.0025 (6)

Geometric parameters (Å, °)

C1—C3^{i}	1.387 (2)	C8—H8A	0.9600
C1—C2	1.3856 (19)	C8—H8B	0.9600
C1—C4	1.5132 (18)	C8—H8C	0.9600
C2—C3	1.388 (2)	N1—H1A	0.882 (9)
C2—H2	0.9300	N2—H2A	0.92 (2)
C3—C1^{i}	1.387 (2)	N3—C9	1.3161 (19)
C3—H3	0.9300	N3—C10	1.377 (2)
C4—O1	1.2497 (18)	N4—C9	1.3428 (19)
C4—O2	1.2526 (17)	N4—C11	1.362 (2)
O3—H3A	0.87 (3)	N4—H4C	0.85 (2)
O3—H3B	0.74 (3)	C9—C12	1.482 (2)
C5—N1	1.323 (2)	C10—C11	1.340 (2)
C5—N2	1.3264 (19)	C10—H10	0.9300
C5—C8	1.479 (2)	C11—H11	0.9300
C6—C7	1.335 (2)	C12—H12A	0.9600
C6—N1	1.373 (2)	C12—H12B	0.9600
C6—H6	0.9300	C12—H12C	0.9600
C7—N2	1.364 (2)	O4—H4A	0.81 (3)
C7—H7	0.9300	O4—H4B	0.90 (3)
C3^{i}—C1—C2	118.56 (12)	H8B—C8—H8C	109.5
C3^{i}—C1—C4	120.37 (12)	C5—N1—C6	108.47 (13)
C2—C1—C4	121.04 (13)	C5—N1—H1A	122.8 (12)
C1—C2—C3	120.78 (14)	C6—N1—H1A	128.7 (12)
C1—C2—H2	119.6	C5—N2—C7	109.04 (14)
C3—C2—H2	119.6	C5—N2—H2A	120.9 (12)
C1^{i}—C3—C2	120.65 (13)	C7—N2—H2A	130.1 (12)
C1^{i}—C3—H3	119.7	C9—N3—C10	105.95 (13)
C2—C3—H3	119.7	C9—N4—C11	108.11 (13)
O1—C4—O2	124.48 (13)	C9—N4—H4C	120.9 (13)
O1—C4—C1	118.14 (12)	C11—N4—H4C	131.0 (13)
O2—C4—C1	117.34 (13)	N3—C9—N4	110.18 (13)
H3A—O3—H3B	102 (3)	N3—C9—C12	125.60 (14)
N1—C5—N2	108.09 (14)	N4—C9—C12	124.22 (14)
N1—C5—C8	126.33 (14)	C11—C10—N3	109.68 (14)
N2—C5—C8	125.58 (14)	C11—C10—H10	125.2
C7—C6—N1	107.40 (15)	N3—C10—H10	125.2
C7—C6—H6	126.3	C10—C11—N4	106.08 (14)
N1—C6—H6	126.3	C10—C11—H11	127.0
C6—C7—N2	106.99 (15)	N4—C11—H11	127.0

C6—C7—H7	126.5	C9—C12—H12A	109.5
N2—C7—H7	126.5	C9—C12—H12B	109.5
C5—C8—H8A	109.5	H12A—C12—H12B	109.5
C5—C8—H8B	109.5	C9—C12—H12C	109.5
H8A—C8—H8B	109.5	H12A—C12—H12C	109.5
C5—C8—H8C	109.5	H12B—C12—H12C	109.5
H8A—C8—H8C	109.5	H4A—O4—H4B	104 (2)

C3^{i}—C1—C2—C3	0.4 (2)	N1—C5—N2—C7	−0.39 (19)
C4—C1—C2—C3	178.32 (12)	C8—C5—N2—C7	179.21 (16)
C1—C2—C3—C1^{i}	−0.4 (2)	C6—C7—N2—C5	−0.1 (2)
C3^{i}—C1—C4—O1	−178.91 (12)	C10—N3—C9—N4	0.36 (17)
C2—C1—C4—O1	3.20 (19)	C10—N3—C9—C12	−178.94 (16)
C3^{i}—C1—C4—O2	3.24 (19)	C11—N4—C9—N3	−0.22 (18)
C2—C1—C4—O2	−174.66 (12)	C11—N4—C9—C12	179.09 (16)
N1—C6—C7—N2	0.4 (2)	C9—N3—C10—C11	−0.36 (18)
N2—C5—N1—C6	0.66 (18)	N3—C10—C11—N4	0.23 (19)
C8—C5—N1—C6	−178.92 (16)	C9—N4—C11—C10	−0.01 (19)
C7—C6—N1—C5	−0.7 (2)		

Symmetry codes: (i) $-x$, $-y$, $-z+1$.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1A···N3	0.882 (9)	1.830 (10)	2.7078 (18)	173.5 (17)
N2—H2A···O2	0.92 (2)	1.78 (2)	2.6965 (17)	175.6 (17)
O3—H3B···O1	0.74 (3)	2.08 (3)	2.8138 (18)	170 (3)
O4—H4B···O1	0.90 (3)	1.87 (3)	2.7723 (17)	175 (2)
O3—H3A···O2^{ii}	0.87 (3)	1.94 (3)	2.812 (2)	176 (3)
O4—H4A···O3^{iii}	0.81 (3)	1.97 (3)	2.766 (2)	166 (3)
N4—H4C···O4^{iv}	0.85 (2)	1.94 (2)	2.7872 (19)	175.7 (18)
C12—H12B···O3^{v}	0.96	2.59	3.542 (2)	169
C10—H10···Cg^{vi}	0.93	2.89	3.700 (2)	147

Symmetry codes: (ii) $x+1$, y, z; (iii) $-x+1$, $-y$, $-z$; (iv) $-x$, $-y+1$, $-z-1$; (v) $x-1$, $y+1$, $z-1$; (vi) x, y, $z-1$.

Fig. 1

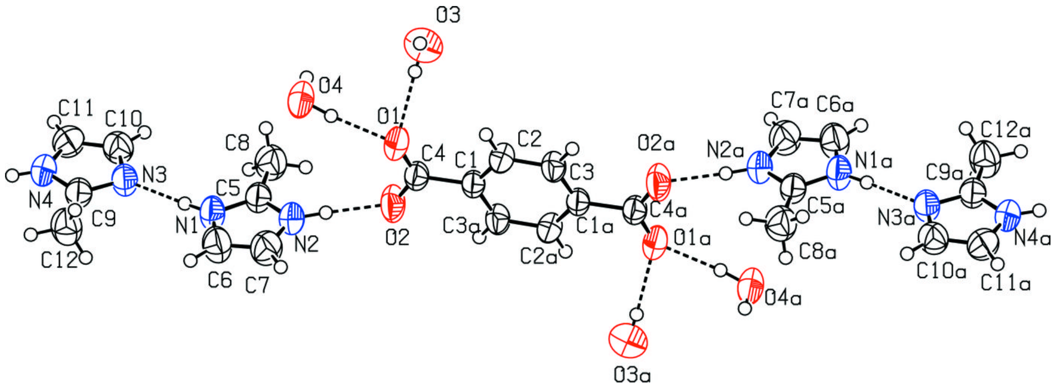
O3
O4
O1
C11
C10
C8
C4
C1
C2
N3
C5
C3
O2a
N2a
C7a
C6a
C12a
N1a
C9a
N4
C9
N1
N2
O2
C3a
C2a
C1a
C4a
O1a
C5a
C8a
N3a
N4a
C12
C6
C7
C10a
C11a
O4a
O3a

Fig. 2

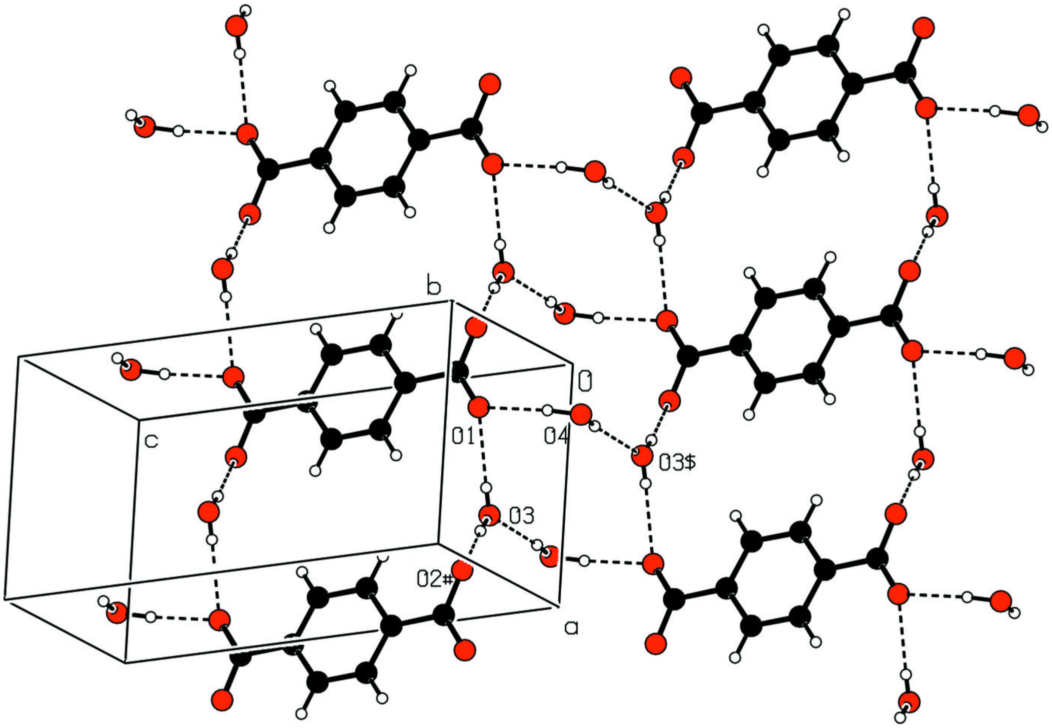

Fig. 3