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Synthesis and structure of 3-methylpyridinium 3-carboxy-5-nitrobenzoate monohydrate

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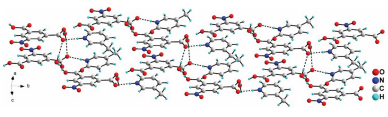
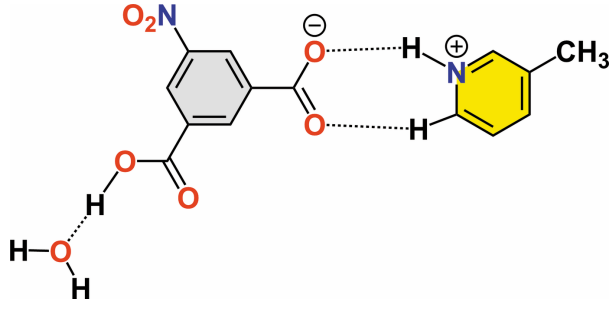
The title compound, $C_6H_8N^+\cdot C_8H_4NO_6^-\cdot H_2O$, crystallizes in the monoclinic crystal space group $C2/c$. An N—H···O hydrogen bond is observed between the 3-methylpyridinium cation and the 5-nitroisophthalate anion. The crystal packing is consolidated by an extensive network of intermolecular O—H···O, N—H···O, and C—H···O hydrogen bonds, further reinforced by π–π interactions.

1. Chemical context

Co-crystals are homogeneous crystalline solids composed of two or more neutral components in definite stoichiometric ratios, assembled under ambient conditions through non-covalent interactions such as hydrogen bonding, π–π stacking, and van der Waals forces (Pan *et al.*, 2019). The key distinction between a co-crystal and a salt lies in the position of the acidic proton within the acid–base pair. When proton transfer to the base is complete, salt formation is favoured over co-crystal formation. The acidity of aromatic acids, and hence their proton-donating ability, is strongly influenced by the nature and position of substituents on the aromatic ring. Electron-withdrawing groups tend to enhance acidity, whereas electron-donating groups reduce it. Consequently, the tendency of a hydrogen-bond acceptor to form either a co-crystal or a salt depends significantly on these substituent effects.

Previous studies by Mohamed *et al.* (2009) have highlighted the role of pyridine–carboxylic acid and pyridinium–carboxylate synthons in governing the crystal packing of binary solid systems. In addition, our group has reported co-crystals of gallic acid with 4-cyanopyridine, demonstrating the significance of O—H···N intermolecular hydrogen bonding in consolidating the structure (Goswami *et al.*, 2021). Another study from our group describes the crystal structure of phenylenediacetic acid with 4,4′-bipyridine, where similar hydrogen-bonding motifs, including O—H···N, C—H···N, and C—H···π interactions, play a crucial role in consolidating the solid-state architecture (Paul & Bora, 2015).





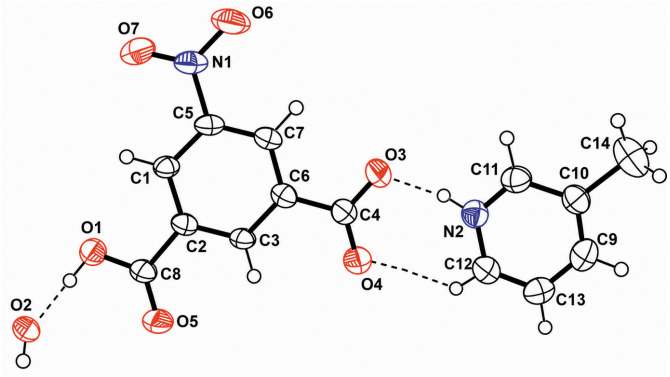


Figure 1
The molecular structure of the title compound with displacement ellipsoids drawn at 50% probability. All the non H-atoms are labelled. The dashed lines depict hydrogen bonds.

2. Structural commentary

The title hydrated salt (Fig. 1) crystallizes in the monoclinic crystal system with the space group *C*2/*c*. In this structure, 3-methylpyridine accepts a proton from 5-nitroisophthalic acid, resulting in the formation of a pyridinium cation. The protonated base and the corresponding carboxylate anion together constitute a salt, consolidated by N—H···O and C—H···O hydrogen bonds, which can be described by the graph-set motif $R_2^2(7)$. In addition, the water molecule of crystallization participates in an extended hydrogen-bonding network with the 5-nitroisophthalate moiety, further reinforcing the supramolecular assembly. Analysis of the difference-Fourier map reveals positive electron density near the nitrogen atom (N2) at a distance of 0.88 (3) Å, consistent with a typical Nsp^2—H bond length. Additionally, a negative residual electron density peak is observed near the O3 atom, indicating proton transfer between the acid and pyridine components. Consequently, the pyridinium cation is consolidated by the carboxylate anion through strong hydrogen bonding, leading to the formulation of the compound as a hydrated salt, $C_6H_8N^+C_8H_4NO_6{\cdot}H_2O$.

3. Supramolecular features

The water molecule of crystallization further acts as a hydrogen-bond donor through the O2—H2*A*···O4 interaction [O···O = 2.718 (2) Å], linking neighbouring carboxylate groups belonging to adjacent 5-nitroisophthalate units. Consequently, the water molecule functions as a supramolecular bridge, propagating the structure into an extended hydrogen-bonded chain running through the crystal structure (Table 1, Fig. 2). The hydrogen-bonded chains are further interconnected through electrostatic interactions between the protonated 3-methylpyridinium cations and the negatively charged 5-nitroisophthalate anions. Additional weak C—H···O contacts involving pyridinium and aromatic C—H donors with carboxylate and nitro oxygen atom acceptors reinforce these connections, leading to the formation of extended supramolecular sheets (Fig. 3). Beyond hydrogen bonding, the crystal packing is further consolidated by aromatic π–π stacking interactions between neighbouring pyridinium and benzene rings [*Cg*1···*Cg*1(1 − *x*, *y*,1 /2 − *z*) = 3.7963 (14) Å and *Cg*2···*Cg*2 = 3.5924 (15) Å where *Cg*1 and *Cg*2 are the centroids of the C1–C3/C5–C7 and N2/C9–C13 rings, respectively]. These interactions promote the formation of columnar arrangements along specific crystallographic directions and facilitate efficient molecular packing (Fig. 4). The combined effect of strong O—H···O hydrogen bonds, water-mediated bridges, weak C—H···O interactions and π–π interactions ultimately generates a highly interconnected three-dimensional network. Thus, the crystal structure may be viewed as a hydrogen-bond-directed framework in which water molecules of crystallization play a central structure-directing role, while aromatic stacking interactions provide additional consolidation and packing efficiency.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C12—H12···O4	0.93	2.59	3.201 (3)	124
O1—H1···O2	0.92 (3)	1.64 (3)	2.5473 (19)	170 (3)
N2—H2···O3	0.89 (3)	1.77 (3)	2.643 (2)	171 (3)
O2—H2*A*···O4^{i}	0.84 (2)	1.89 (2)	2.718 (2)	171 (3)
O2—H2*B*···O3^{ii}	0.82 (2)	2.03 (2)	2.829 (2)	163 (3)

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

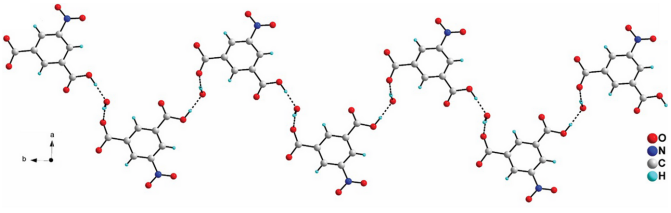


Figure 2
Water-mediated O—H···O linkage showing the chain structure.

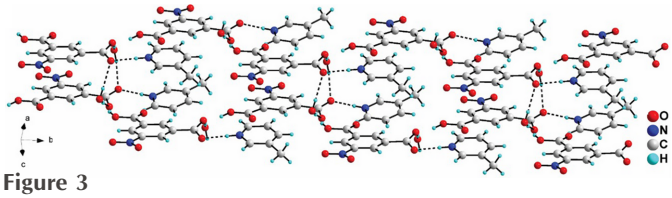


Figure 3
Hydrogen-bonded layer viewed down the *bc* plane.

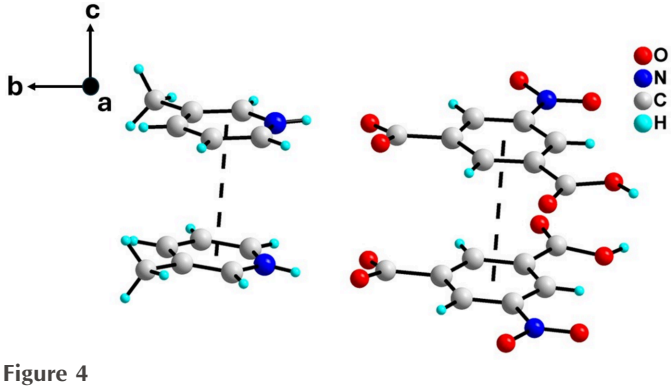


Figure 4
π–π stacking interactions between pyridinium and phenyl rings viewed down the *bc* plane

Table 1 summarizes the hydrogen-bonding parameters. The crystal structure is primarily consolidated by a network of strong and highly directional O—H···O and N—H···O hydrogen bonds, with additional contributions from weaker C—H···O interactions. The O1—H1···O2 and N2—H2···O3 hydrogen bonds exhibit short H···*A* distances [1.64 (3) and 1.77 (3) Å] and nearly linear bond angles [170 (3) and 171 (3)°], indicating their significant role in enhancing the crystal cohesion. Similarly, the O2—H2*A*···O4 interaction displays a near-linear geometry [171 (3)°] with a short H···*A* distance [1.89 (2) Å], further strengthening the supramolecular framework. In contrast, the O2—H2*B*···O3 hydrogen bond is relatively weaker, as evidenced by its longer H···*A* distance [2.03 (2) Å] and slightly reduced bond angle [163 (3)°]. The weakest interaction in the structure is the C12—H12···O4 contact, characterized by a comparatively long H···*A* distance (2.59 Å) and a markedly bent geometry (124°), typical of weak C—H···O interactions.

Thus, the crystal structure develops through a stepwise assembly process: strong O—H···O and N—H···O hydrogen bonds, together with water-mediated bridges, construct the primary chains; weaker C—H···O interactions interconnect these chains into sheets; and finally, π–π interactions reinforce the packing to produce a robust three-dimensional supramolecular architecture.

4. Database survey

While several examples utilizing 3-methylpyridine as a supramolecular synthon have been documented in earlier studies (Trollip *et al.*, 2025; Yamada *et al.*, 2013), no corresponding crystallographic examples employing 5-nitroisophthalic acid as a supramolecular synthon were found in the available literature.

5. Synthesis and crystallization

3-Methylpyridine (1m*M*, 0.0913 g) and 5-nitroisopthalic acid (1m*M*, 0.2111 g) were taken in an oven-dried round-bottom flask. Then 20 mL of water was added and the reaction mixture was refluxed at 373 K for 5h. The resulting solution was then cooled at room temperature and kept undisturbed for crystallization. After a few days, colourless needle-shaped good-quality crystals evolved from the solution.

6. Refinement

Crystal data, data collection parameters, and structure refinement details are compiled in Table 2. The H attached to aromatic carbon atoms were refined with the riding model. The HFIX 43 (one hydrogen on an sp^2-hybridized carbon atom) command was used to add the C-bound hydrogen atoms (C1, C7, C3, C9, C10, C11, C12, C13). Subsequently, the hydrogen atoms on the methyl carbon (C14) of the 3-methylpyridinium cation were added with the help of HFIX 137 (three hydrogen atoms on sp^3-hybridized carbon atom) command and the hydrogen on the nitrogen atom (N2) of the pyridinium cation was found in a difference-Fourier map. The hydrogen atom on the –COOH group (O1) was fixed with HFIX 134 (one hydrogen O—H···H bonded). The hydrogen atoms associated with the water molecule (O2) were identified from difference-Fourier maps and refined using the DFIX command.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_6H_8N^+·C_8H_4NO_6^-·H_2O$
M_r	322.27
Crystal system, space group	Monoclinic, *C*2/*c*
Temperature (K)	296
a, *b*, *c* (Å)	14.001 (4), 14.989 (4), 14.269 (4)
β (°)	94.550 (5)
V (Å^3)	2985.2 (15)
Z	8
Radiation type	Mo *K*α
μ (mm^{-1})	0.12
Crystal size (mm)	0.21 × 0.18 × 0.15
Data collection	
Diffractometer	Bruker APEXII CCD
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	37111, 4407, 3029
R_{int}	0.066
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.709
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.069, 0.181, 1.07
No. of reflections	4407
No. of parameters	225
No. of restraints	2
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.37, −0.49

Computer programs: *APEX2* and *SAINT* (Bruker, 2012), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2019/3* (Sheldrick, 2015*b*) and *OLEX2* (Dolomanov *et al.*, 2009).

Acknowledgements

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Synthesis and structure of 3-methylpyridinium 3-carboxy-5-nitrobenzoate monohydrate

Karmajyoti Borah, Sourajyoti Ray and Sanchay Jyoti Bora

Computing details

3-Methylpyridinium 3-carboxy-5-nitrobenzoate monohydrate

Crystal data

$C_6H_8N^+·C_8H_4NO_6^-·H_2O$
M_r = 322.27
Monoclinic, *C*2/*c*
a = 14.001 (4) Å
b = 14.989 (4) Å
c = 14.269 (4) Å
β = 94.550 (5)°
V = 2985.2 (15) Å^3
Z = 8
F(000) = 1344
D_x = 1.434 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 7138 reflections
θ = 2.4–28.3°
μ = 0.12 mm^{-1}
T = 296 K
Block, colorless
0.21 × 0.18 × 0.15 mm

Data collection

Bruker APEXII CCD diffractometer
φ and *ω* scans
37111 measured reflections
4407 independent reflections
3029 reflections with $I > 2\sigma(I)$
R_{int} = 0.066
θ_{max} = 30.3°, θ_{min} = 3.4°
h = −19→19
k = −21→21
l = −20→20

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.069
$wR(F^2)$ = 0.181
S = 1.07
4407 reflections
225 parameters
2 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.085P)^2 + 1.6623P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.49 e Å^{-3}

Special details

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

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.36724 (9)	−0.07423 (9)	0.32424 (11)	0.0527 (4)
O2	0.21930 (10)	−0.17216 (10)	0.29414 (12)	0.0500 (4)
O3	0.55819 (10)	0.36420 (9)	0.39569 (11)	0.0529 (4)
O4	0.40090 (10)	0.34674 (10)	0.36377 (11)	0.0571 (4)
O5	0.27850 (10)	0.04296 (10)	0.27574 (13)	0.0628 (4)
O6	0.74673 (9)	0.09885 (12)	0.49234 (12)	0.0647 (5)
O7	0.69029 (11)	−0.03206 (12)	0.46412 (14)	0.0735 (5)
N1	0.68314 (10)	0.04850 (12)	0.46136 (11)	0.0457 (4)
N2	0.50959 (13)	0.53448 (12)	0.38409 (12)	0.0471 (4)
C1	0.52059 (11)	0.03101 (12)	0.38648 (11)	0.0352 (4)
H1A	0.528922	−0.030520	0.388917	0.042*
C2	0.43451 (10)	0.06861 (11)	0.34855 (11)	0.0334 (3)
C3	0.42381 (11)	0.16076 (12)	0.34615 (11)	0.0348 (3)
H3	0.366433	0.185404	0.321000	0.042*
C4	0.48381 (12)	0.31673 (12)	0.37892 (12)	0.0401 (4)
C5	0.59294 (10)	0.08824 (12)	0.42025 (11)	0.0357 (4)
C6	0.49779 (11)	0.21682 (11)	0.38085 (11)	0.0349 (3)
C7	0.58390 (11)	0.17971 (12)	0.41832 (11)	0.0372 (4)
H7	0.634195	0.216028	0.441536	0.045*
C8	0.35184 (11)	0.01167 (12)	0.31163 (13)	0.0383 (4)
C9	0.47158 (15)	0.71004 (14)	0.36545 (14)	0.0517 (5)
H9	0.457902	0.770547	0.359053	0.062*
C10	0.56465 (14)	0.68319 (14)	0.39173 (13)	0.0480 (4)
C11	0.58072 (14)	0.59327 (15)	0.40111 (14)	0.0492 (5)
H11	0.642054	0.572838	0.419599	0.059*
C12	0.41998 (14)	0.55942 (15)	0.35814 (14)	0.0518 (5)
H12	0.372180	0.516842	0.346604	0.062*
C13	0.39898 (15)	0.64855 (16)	0.34863 (15)	0.0548 (5)
H13	0.336755	0.667193	0.331114	0.066*
C14	0.6452 (2)	0.7490 (2)	0.4071 (2)	0.0827 (8)
H14A	0.644178	0.789193	0.354609	0.124*
H14B	0.705225	0.717712	0.412902	0.124*
H14C	0.637817	0.782262	0.463557	0.124*
H1	0.3152 (19)	−0.1097 (19)	0.3067 (18)	0.075 (8)*
H2	0.530 (2)	0.479 (2)	0.3936 (19)	0.083 (9)*
H2A	0.1873 (18)	−0.1635 (19)	0.2430 (14)	0.075 (8)*
H2B	0.1809 (19)	−0.159 (2)	0.3326 (18)	0.092 (11)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0311 (6)	0.0382 (7)	0.0865 (10)	−0.0059 (5)	−0.0099 (6)	0.0024 (7)
O2	0.0347 (7)	0.0438 (8)	0.0702 (10)	−0.0086 (6)	−0.0046 (7)	−0.0031 (7)
O3	0.0390 (7)	0.0399 (7)	0.0783 (10)	−0.0051 (5)	−0.0051 (6)	−0.0077 (6)
O4	0.0409 (7)	0.0478 (8)	0.0804 (10)	0.0050 (6)	−0.0088 (7)	−0.0075 (7)

O5	0.0370 (7)	0.0507 (8)	0.0956 (12)	−0.0054 (6)	−0.0263 (7)	0.0071 (8)
O6	0.0325 (7)	0.0790 (11)	0.0792 (10)	−0.0080 (7)	−0.0165 (6)	0.0071 (8)
O7	0.0457 (8)	0.0580 (10)	0.1124 (15)	0.0083 (7)	−0.0217 (8)	0.0134 (9)
N1	0.0265 (7)	0.0600 (11)	0.0494 (9)	−0.0013 (7)	−0.0037 (6)	0.0095 (7)
N2	0.0512 (9)	0.0401 (9)	0.0500 (9)	0.0037 (7)	0.0034 (7)	−0.0019 (7)
C1	0.0272 (7)	0.0382 (9)	0.0401 (8)	−0.0012 (6)	0.0015 (6)	0.0047 (6)
C2	0.0238 (7)	0.0402 (9)	0.0358 (8)	−0.0044 (6)	0.0000 (6)	0.0009 (6)
C3	0.0238 (7)	0.0408 (9)	0.0392 (8)	0.0002 (6)	−0.0011 (6)	−0.0003 (6)
C4	0.0371 (8)	0.0389 (9)	0.0435 (9)	−0.0010 (7)	−0.0020 (7)	−0.0047 (7)
C5	0.0226 (7)	0.0482 (10)	0.0359 (8)	−0.0004 (6)	−0.0003 (5)	0.0058 (7)
C6	0.0295 (7)	0.0384 (9)	0.0365 (8)	−0.0032 (6)	0.0010 (6)	−0.0019 (6)
C7	0.0274 (7)	0.0467 (10)	0.0368 (8)	−0.0067 (7)	−0.0011 (6)	−0.0001 (7)
C8	0.0264 (7)	0.0404 (9)	0.0472 (9)	−0.0048 (6)	−0.0018 (6)	0.0007 (7)
C9	0.0608 (12)	0.0431 (11)	0.0515 (11)	0.0076 (9)	0.0064 (9)	0.0019 (8)
C10	0.0490 (10)	0.0511 (11)	0.0442 (9)	−0.0054 (9)	0.0061 (8)	−0.0051 (8)
C11	0.0411 (9)	0.0563 (12)	0.0499 (10)	0.0074 (8)	0.0008 (7)	−0.0039 (9)
C12	0.0464 (10)	0.0548 (12)	0.0536 (11)	−0.0066 (9)	0.0001 (8)	−0.0025 (9)
C13	0.0440 (10)	0.0622 (13)	0.0573 (12)	0.0091 (9)	−0.0021 (8)	0.0054 (9)
C14	0.0750 (17)	0.0785 (19)	0.095 (2)	−0.0280 (15)	0.0090 (14)	−0.0142 (15)

Geometric parameters (Å, º)

O1—C8	1.315 (2)	C3—H3	0.9300
O1—H1	0.92 (3)	C3—C6	1.394 (2)
O2—H2A	0.836 (17)	C4—C6	1.510 (3)
O2—H2B	0.822 (18)	C5—C7	1.377 (3)
O3—C4	1.268 (2)	C6—C7	1.395 (2)
O4—C4	1.248 (2)	C7—H7	0.9300
O5—C8	1.206 (2)	C9—H9	0.9300
O6—N1	1.223 (2)	C9—C10	1.387 (3)
O7—N1	1.212 (2)	C9—C13	1.379 (3)
N1—C5	1.475 (2)	C10—C11	1.371 (3)
N2—C11	1.337 (3)	C10—C14	1.502 (3)
N2—C12	1.333 (3)	C11—H11	0.9300
N2—H2	0.89 (3)	C12—H12	0.9300
C1—H1A	0.9300	C12—C13	1.372 (3)
C1—C2	1.400 (2)	C13—H13	0.9300
C1—C5	1.384 (2)	C14—H14A	0.9600
C2—C3	1.390 (2)	C14—H14B	0.9600
C2—C8	1.500 (2)	C14—H14C	0.9600
C8—O1—H1	114.3 (17)	C5—C7—H7	120.7
H2A—O2—H2B	102 (3)	C6—C7—H7	120.7
O6—N1—C5	118.06 (17)	O1—C8—C2	113.28 (14)
O7—N1—O6	123.18 (16)	O5—C8—O1	124.32 (16)
O7—N1—C5	118.75 (15)	O5—C8—C2	122.38 (16)
C11—N2—H2	111.7 (19)	C10—C9—H9	119.4
C12—N2—C11	122.44 (19)	C13—C9—H9	119.4

C12—N2—H2	125.9 (19)	C13—C9—C10	121.1 (2)
C2—C1—H1A	121.0	C9—C10—C14	121.8 (2)
C5—C1—H1A	121.0	C11—C10—C9	117.07 (19)
C5—C1—C2	117.96 (16)	C11—C10—C14	121.1 (2)
C1—C2—C8	121.58 (15)	N2—C11—C10	121.05 (18)
C3—C2—C1	119.83 (14)	N2—C11—H11	119.5
C3—C2—C8	118.58 (14)	C10—C11—H11	119.5
C2—C3—H3	119.5	N2—C12—H12	120.3
C2—C3—C6	120.99 (14)	N2—C12—C13	119.34 (19)
C6—C3—H3	119.5	C13—C12—H12	120.3
O3—C4—C6	116.71 (15)	C9—C13—H13	120.5
O4—C4—O3	124.70 (17)	C12—C13—C9	118.95 (19)
O4—C4—C6	118.55 (15)	C12—C13—H13	120.5
C1—C5—N1	117.90 (16)	C10—C14—H14A	109.5
C7—C5—N1	118.97 (14)	C10—C14—H14B	109.5
C7—C5—C1	123.13 (14)	C10—C14—H14C	109.5
C3—C6—C4	119.98 (14)	H14A—C14—H14B	109.5
C3—C6—C7	119.40 (16)	H14A—C14—H14C	109.5
C7—C6—C4	120.61 (14)	H14B—C14—H14C	109.5
C5—C7—C6	118.68 (14)		

O3—C4—C6—C3	−167.89 (16)	C2—C3—C6—C4	−178.98 (15)
O3—C4—C6—C7	13.0 (2)	C2—C3—C6—C7	0.2 (2)
O4—C4—C6—C3	14.0 (2)	C3—C2—C8—O1	−174.88 (15)
O4—C4—C6—C7	−165.10 (16)	C3—C2—C8—O5	3.8 (3)
O6—N1—C5—C1	−179.09 (16)	C3—C6—C7—C5	−0.3 (2)
O6—N1—C5—C7	0.0 (2)	C4—C6—C7—C5	178.82 (15)
O7—N1—C5—C1	−0.1 (2)	C5—C1—C2—C3	−0.3 (2)
O7—N1—C5—C7	178.97 (18)	C5—C1—C2—C8	−179.11 (15)
N1—C5—C7—C6	−178.88 (14)	C8—C2—C3—C6	179.00 (15)
N2—C12—C13—C9	0.6 (3)	C9—C10—C11—N2	1.0 (3)
C1—C2—C3—C6	0.1 (2)	C10—C9—C13—C12	−0.1 (3)
C1—C2—C8—O1	4.0 (2)	C11—N2—C12—C13	−0.2 (3)
C1—C2—C8—O5	−177.31 (18)	C12—N2—C11—C10	−0.6 (3)
C1—C5—C7—C6	0.2 (2)	C13—C9—C10—C11	−0.7 (3)
C2—C1—C5—N1	179.19 (14)	C13—C9—C10—C14	177.9 (2)
C2—C1—C5—C7	0.1 (2)	C14—C10—C11—N2	−177.5 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C12—H12···O4	0.93	2.59	3.201 (3)	124
O1—H1···O2	0.92 (3)	1.64 (3)	2.5473 (19)	170 (3)
N2—H2···O3	0.89 (3)	1.77 (3)	2.643 (2)	171 (3)
O2—H2*A*···O4^{i}	0.84 (2)	1.89 (2)	2.718 (2)	171 (3)
O2—H2*B*···O3^{ii}	0.82 (2)	2.03 (2)	2.829 (2)	163 (3)

Symmetry codes: (i) −*x*+1/2, *y*−1/2, −*z*+1/2; (ii) *x*−1/2, *y*−1/2, *z*.