

Crystal structure of 4-(dimethylamino)-pyridinium 4-aminobenzoate dihydrate

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Received 29 November 2014; accepted 30 November 2014

Edited by W. T. A. Harrison, University of Aberdeen, Scotland

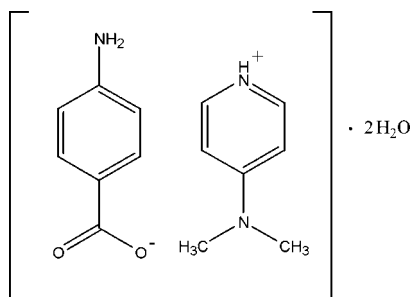
In the title hydrated molecular salt, $C_7H_{11}N_2^+ \cdot C_7H_6NO_2^- \cdot 2H_2O$, the cation is protonated at the pyridine N atom and the dihedral angle between the benzene ring and the CO_2^- group in the anion is $8.5(2)^\circ$. In the crystal, the cation forms an $N-H \cdots O$ hydrogen bond to the anion and the anion forms two $N-H \cdots O$ hydrogen bonds to adjacent water molecules. Both water molecules form two $O-H \cdots O$ hydrogen bonds to carboxylate O atoms. In combination, these hydrogen bonds generate a three-dimensional network and two weak $C-H \cdots \pi$ interactions are also observed.

Keywords: crystal structure; 4-(dimethylamino)pyridinium; 4-aminobenzoate; hydrate; hydrogen bonding.

CCDC reference: 1036769

1. Related literature

For related structures, see: Dhanabalan *et al.* (2014); Lo & Ng (2008); Pereira Silva *et al.* (2010); Sivakumar *et al.* (2014).



2. Experimental

2.1. Crystal data

$C_7H_{11}N_2^+ \cdot C_7H_6NO_2^- \cdot 2H_2O$
 $M_r = 295.34$
 Triclinic, $P\bar{1}$
 $a = 9.3402(7) \text{ \AA}$
 $b = 9.7999(7) \text{ \AA}$
 $c = 10.2132(8) \text{ \AA}$
 $\alpha = 65.755(3)^\circ$
 $\beta = 69.983(2)^\circ$

$\gamma = 89.212(3)^\circ$
 $V = 792.08(10) \text{ \AA}^3$
 $Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 0.09 \text{ mm}^{-1}$
 $T = 295 \text{ K}$
 $0.30 \times 0.24 \times 0.20 \text{ mm}$

2.2. Data collection

Bruker Kappa APEXII CCD diffractometer
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.973$, $T_{\max} = 0.982$

16983 measured reflections
 3337 independent reflections
 2141 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.025$

2.3. Refinement

$R[F^2 > 2\sigma(F^2)] = 0.054$
 $wR(F^2) = 0.168$
 $S = 1.03$
 3337 reflections
 216 parameters
 7 restraints

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\max} = 0.29 \text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.23 \text{ e \AA}^{-3}$

Table 1

Hydrogen-bond geometry (\AA , $^\circ$).

Cg_2 is the centroid of the C1–C6 benzene ring.

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$N1-H1A \cdots O3^i$	0.87 (1)	2.04 (1)	2.898 (3)	167 (2)
$N1-H1B \cdots O4^i$	0.89 (1)	2.04 (1)	2.921 (3)	174 (2)
$N2-H2A \cdots O1^{ii}$	0.89 (1)	1.81 (1)	2.697 (2)	174 (2)
$O3-H3A \cdots O2^{iii}$	0.83 (1)	2.03 (1)	2.858 (3)	175 (4)
$O3-H3B \cdots O1^{iv}$	0.83 (1)	2.04 (1)	2.861 (3)	174 (4)
$O4-H4A \cdots O2^v$	0.82 (1)	2.01 (1)	2.834 (3)	175 (4)
$O4-H4B \cdots O1^{vi}$	0.82 (1)	2.04 (1)	2.847 (3)	167 (4)
$C9-H9 \cdots Cg_2^{vii}$	0.93	2.80	3.510 (3)	134
$C12-H12 \cdots Cg_2^i$	0.93	2.84	3.535 (3)	132

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $x, y-1, z+1$; (iii) $-x+1, -y+2, -z$; (iv) $x+1, y, z$; (v) $x, y, z+1$; (vi) $-x+1, -y+2, -z+1$; (vii) $-x, -y+1, -z+1$.

Data collection: APEX2 (Bruker, 2004); cell refinement: SAINT (Bruker, 2004); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: PLATON (Spek, 2009); software used to prepare material for publication: SHELXL97.

Acknowledgements

The authors thank SAIF, IIT, Madras for the data collection.

Supporting information for this paper is available from the IUCr electronic archives (Reference: HB7333).

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supporting information

Acta Cryst. (2015). E71, o26–o27 [https://doi.org/10.1107/S2056989014026310]

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S1. Chemical context

We hereby report the synthesis and crystal structure of the title compound (I), prepared by the reaction of 4-dimethylaminopyridine with 4-aminobenzoic acid in distilled water as solvent.

S2. Structural commentary

The geometric parameters of the title compound (I) (Fig.1) are comparable with the reported structures [Dhanabalan *et al.*, 2014; Lo & Ng (2008); Pereira Silva *et al.*, 2010; Sivakumar *et al.*, 2014]. The 4-dimethylaminopyridinium cation is protonated at pyridine N2 atom, with the plane of the hetro atoms N(CH3)2 (N3/C13/C14) is inclined to the pyridine ring by 4.7 (2)°. In the 4-aminobenzoate anion, the plane of carboxylate group (C7/O1/O2) is skewed at an angle of 8.5 (2)° with the attached benzene ring (C1—C6). The dihedral angle between the benzene ring (C1—C6) and pyridine ring (N2/C8—C12) is 66.69 (8)°.

S3. Supramolecular features

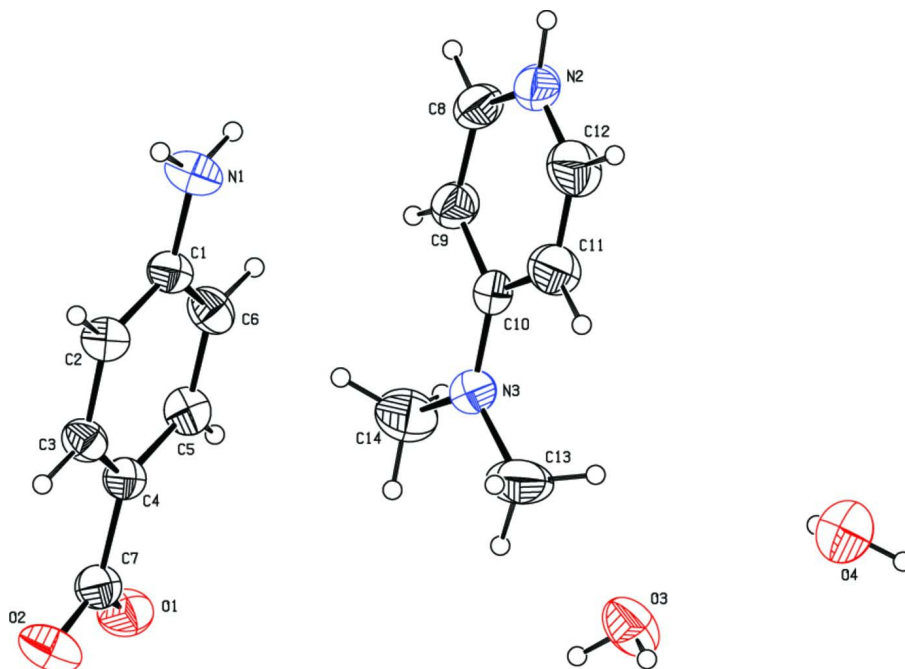
In the crystal, the medium-strength N—H...O and O—H...O hydrogen bonds connect the adjacent anions and cations, involving water molecules into three dimensional framework (Table 2 & Fig. 2). The crystal structure also features weak C—H... π (Table 2) interactions.

S4. Synthesis and crystallization

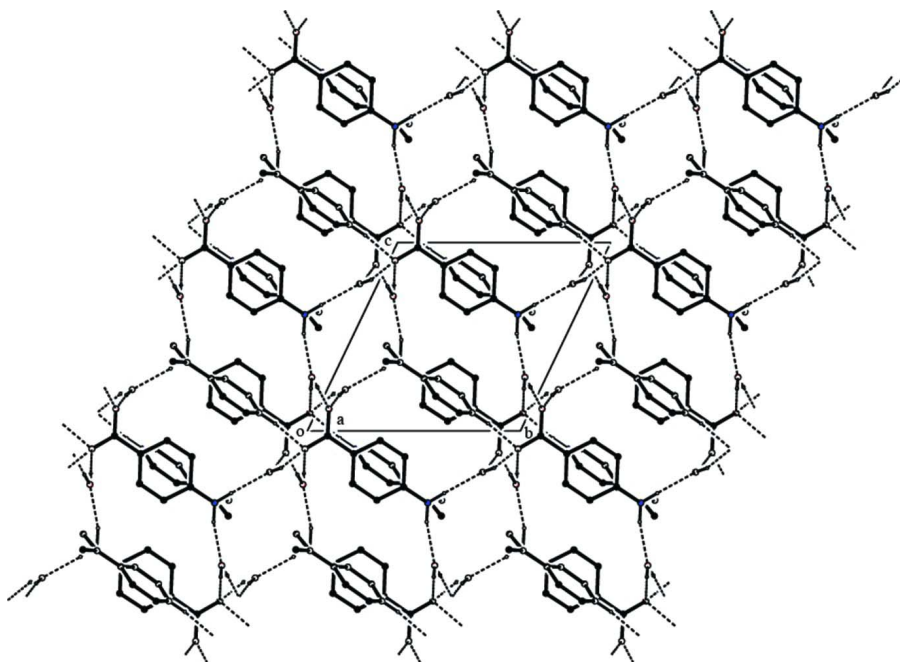
4-Dimethylaminopyridine (C₇H₁₀N₂, 1.9704 g) and 4-aminobenzoic acid (C₇H₇NO₂, 2.2119 g) were taken in the equimolar ratio and synthesized in distilled water and prepared solution was allowed for slow evaporation at room temperature. Colourless blocks were collected after 20 days.

S5. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. The C-bound H atoms were positioned geometrically and refined using riding model, with C—H = 0.93 and 0.97 Å for CH_{aromatic} and CH₃, respectively, with U_{iso}(H) = 1.2Ueq(C) or 1.5Ueq(C). The H atoms bound to O and N atoms were found in a difference map and refined isotropically, with U_{iso}(H) = 1.5Ueq(O). The distance restraints O—H = 0.82 (1)Å and N—H = 0.88 (1)Å were applied during refinement.

**Figure 1**

The molecular structure of (I), with 30% probability displacement ellipsoids for non-H atoms.

**Figure 2**

The packing of (I), viewed down a axis. Intermolecular Hydrogen bonds are shown as dashed lines. H atoms not involved in hydrogen bonding have been omitted.

4-(Dimethylamino)pyridinium 4-aminobenzoate dihydrate

Crystal data

C₇H₁₁N₂⁺·C₇H₆NO₂⁻·2H₂O $M_r = 295.34$ Triclinic, $P\bar{1}$

Hall symbol: -P 1

 $a = 9.3402$ (7) Å $b = 9.7999$ (7) Å $c = 10.2132$ (8) Å $\alpha = 65.755$ (3)° $\beta = 69.983$ (2)° $\gamma = 89.212$ (3)° $V = 792.08$ (10) Å³ $Z = 2$ $F(000) = 316$ $D_x = 1.238$ Mg m⁻³Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 1058 reflections

 $\theta = 2.3$ – 26.7 ° $\mu = 0.09$ mm⁻¹ $T = 295$ K

Block, colourless

 $0.30 \times 0.24 \times 0.20$ mm

Data collection

Bruker Kappa APEXII CCD

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

 ω and ϕ scan

Absorption correction: multi-scan

(SADABS; Sheldrick, 1996)

 $T_{\min} = 0.973$, $T_{\max} = 0.982$

16983 measured reflections

3337 independent reflections

2141 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.025$ $\theta_{\text{max}} = 26.7$ °, $\theta_{\text{min}} = 2.3$ ° $h = -11 \rightarrow 11$ $k = -12 \rightarrow 12$ $l = -12 \rightarrow 12$

Refinement

Refinement on F^2

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.054$ $wR(F^2) = 0.168$ $S = 1.03$

3337 reflections

216 parameters

7 restraints

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

 $w = 1/[\sigma^2(F_o^2) + (0.0709P)^2 + 0.2681P]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\text{max}} < 0.001$ $\Delta\rho_{\text{max}} = 0.29$ e Å⁻³ $\Delta\rho_{\text{min}} = -0.23$ 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.

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 $F^2 > 2\sigma(F^2)$ 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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.2531 (2)	0.4227 (2)	0.2980 (2)	0.0514 (5)
C2	0.3081 (2)	0.4846 (2)	0.1370 (2)	0.0542 (5)
H2	0.3434	0.4230	0.0871	0.065*

C3	0.3104 (2)	0.6362 (2)	0.0517 (2)	0.0531 (5)
H3	0.3492	0.6757	-0.0556	0.064*
C4	0.2567 (2)	0.7315 (2)	0.1210 (2)	0.0491 (4)
C5	0.2008 (2)	0.6690 (2)	0.2806 (2)	0.0568 (5)
H5	0.1630	0.7305	0.3302	0.068*
C6	0.1998 (2)	0.5183 (2)	0.3680 (2)	0.0581 (5)
H6	0.1631	0.4799	0.4751	0.070*
C7	0.2563 (2)	0.8938 (2)	0.0265 (3)	0.0577 (5)
C8	0.1012 (3)	0.3280 (2)	0.9041 (3)	0.0708 (6)
H8	0.0065	0.2666	0.9669	0.085*
C9	0.1039 (3)	0.4747 (2)	0.8167 (3)	0.0655 (6)
H9	0.0118	0.5130	0.8197	0.079*
C10	0.2434 (3)	0.5707 (2)	0.7214 (3)	0.0622 (6)
C11	0.3751 (3)	0.5037 (3)	0.7234 (3)	0.0903 (9)
H11	0.4716	0.5621	0.6622	0.108*
C12	0.3649 (3)	0.3550 (3)	0.8129 (3)	0.0892 (8)
H12	0.4546	0.3123	0.8114	0.107*
C13	0.3933 (4)	0.8197 (4)	0.5480 (5)	0.159 (2)
H13A	0.4464	0.8139	0.6153	0.238*
H13B	0.3738	0.9215	0.5003	0.238*
H13C	0.4557	0.7910	0.4695	0.238*
C14	0.1109 (4)	0.7869 (3)	0.6311 (4)	0.1021 (10)
H14A	0.0473	0.7295	0.6093	0.153*
H14B	0.1394	0.8888	0.5515	0.153*
H14C	0.0548	0.7877	0.7290	0.153*
N1	0.2553 (2)	0.2736 (2)	0.3824 (2)	0.0707 (5)
H1A	0.218 (3)	0.236 (3)	0.4832 (12)	0.078 (8)*
H1B	0.282 (3)	0.218 (3)	0.331 (3)	0.082 (8)*
N2	0.2282 (2)	0.2677 (2)	0.9039 (2)	0.0694 (5)
H2A	0.218 (3)	0.1687 (12)	0.961 (2)	0.079 (7)*
N3	0.2487 (3)	0.7185 (2)	0.6365 (3)	0.0864 (7)
O1	0.18777 (18)	0.97118 (16)	0.09587 (19)	0.0718 (5)
O2	0.3219 (2)	0.94822 (18)	-0.1168 (2)	0.0820 (5)
O3	0.8669 (2)	0.9002 (3)	0.2848 (2)	0.0923 (6)
H3A	0.816 (4)	0.948 (4)	0.233 (4)	0.138*
H3B	0.9578 (17)	0.921 (4)	0.225 (4)	0.138*
O4	0.6374 (2)	0.9148 (2)	0.7810 (3)	0.0908 (6)
H4A	0.5475 (17)	0.930 (4)	0.810 (4)	0.136*
H4B	0.693 (4)	0.960 (4)	0.803 (4)	0.136*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0425 (10)	0.0498 (10)	0.0531 (11)	0.0097 (8)	-0.0151 (8)	-0.0161 (9)
C2	0.0508 (11)	0.0528 (11)	0.0534 (11)	0.0106 (8)	-0.0121 (9)	-0.0236 (9)
C3	0.0493 (11)	0.0562 (11)	0.0442 (10)	0.0081 (8)	-0.0124 (8)	-0.0168 (9)
C4	0.0419 (10)	0.0491 (10)	0.0529 (11)	0.0087 (8)	-0.0171 (8)	-0.0194 (9)
C5	0.0549 (11)	0.0607 (12)	0.0589 (12)	0.0174 (9)	-0.0196 (9)	-0.0310 (10)

C6	0.0560 (12)	0.0667 (13)	0.0444 (11)	0.0145 (9)	-0.0153 (9)	-0.0202 (9)
C7	0.0482 (11)	0.0525 (11)	0.0687 (14)	0.0109 (9)	-0.0246 (10)	-0.0206 (10)
C8	0.0618 (13)	0.0555 (12)	0.0919 (17)	0.0015 (10)	-0.0354 (12)	-0.0230 (12)
C9	0.0616 (13)	0.0575 (12)	0.0797 (15)	0.0095 (10)	-0.0316 (11)	-0.0273 (11)
C10	0.0718 (14)	0.0553 (12)	0.0667 (13)	0.0014 (10)	-0.0410 (11)	-0.0202 (10)
C11	0.0593 (14)	0.0892 (18)	0.0937 (19)	-0.0039 (13)	-0.0376 (14)	-0.0048 (15)
C12	0.0643 (15)	0.0915 (19)	0.103 (2)	0.0203 (14)	-0.0437 (15)	-0.0234 (16)
C13	0.131 (3)	0.092 (2)	0.177 (4)	-0.044 (2)	-0.096 (3)	0.046 (2)
C14	0.130 (3)	0.0622 (15)	0.120 (3)	0.0295 (16)	-0.064 (2)	-0.0303 (16)
N1	0.0811 (13)	0.0549 (11)	0.0565 (12)	0.0159 (9)	-0.0167 (10)	-0.0130 (9)
N2	0.0796 (14)	0.0520 (10)	0.0877 (14)	0.0123 (10)	-0.0473 (11)	-0.0274 (10)
N3	0.0961 (16)	0.0599 (12)	0.0969 (16)	-0.0098 (11)	-0.0602 (13)	-0.0074 (11)
O1	0.0744 (10)	0.0538 (8)	0.0866 (11)	0.0189 (7)	-0.0286 (9)	-0.0308 (8)
O2	0.0879 (12)	0.0644 (10)	0.0658 (11)	0.0250 (8)	-0.0198 (9)	-0.0095 (8)
O3	0.0898 (13)	0.1101 (15)	0.0598 (11)	0.0207 (12)	-0.0261 (9)	-0.0222 (10)
O4	0.0835 (13)	0.1013 (14)	0.1038 (14)	0.0223 (11)	-0.0322 (12)	-0.0615 (12)

Geometric parameters (Å, °)

C1—N1	1.362 (3)	C10—C11	1.389 (3)
C1—C6	1.389 (3)	C11—C12	1.348 (4)
C1—C2	1.395 (3)	C11—H11	0.9300
C2—C3	1.375 (3)	C12—N2	1.338 (3)
C2—H2	0.9300	C12—H12	0.9300
C3—C4	1.383 (3)	C13—N3	1.446 (4)
C3—H3	0.9300	C13—H13A	0.9600
C4—C5	1.383 (3)	C13—H13B	0.9600
C4—C7	1.484 (3)	C13—H13C	0.9600
C5—C6	1.375 (3)	C14—N3	1.451 (4)
C5—H5	0.9300	C14—H14A	0.9600
C6—H6	0.9300	C14—H14B	0.9600
C7—O2	1.248 (3)	C14—H14C	0.9600
C7—O1	1.267 (3)	N1—H1A	0.874 (10)
C8—N2	1.318 (3)	N1—H1B	0.885 (10)
C8—C9	1.341 (3)	N2—H2A	0.890 (10)
C8—H8	0.9300	O3—H3A	0.826 (10)
C9—C10	1.394 (3)	O3—H3B	0.825 (10)
C9—H9	0.9300	O4—H4A	0.823 (10)
C10—N3	1.339 (3)	O4—H4B	0.821 (10)
N1—C1—C6	121.60 (19)	C12—C11—C10	120.8 (2)
N1—C1—C2	120.45 (18)	C12—C11—H11	119.6
C6—C1—C2	117.94 (17)	C10—C11—H11	119.6
C3—C2—C1	120.44 (18)	N2—C12—C11	121.3 (2)
C3—C2—H2	119.8	N2—C12—H12	119.3
C1—C2—H2	119.8	C11—C12—H12	119.3
C2—C3—C4	121.77 (18)	N3—C13—H13A	109.5
C2—C3—H3	119.1	N3—C13—H13B	109.5

C4—C3—H3	119.1	H13A—C13—H13B	109.5
C3—C4—C5	117.50 (17)	N3—C13—H13C	109.5
C3—C4—C7	120.77 (18)	H13A—C13—H13C	109.5
C5—C4—C7	121.72 (18)	H13B—C13—H13C	109.5
C6—C5—C4	121.59 (19)	N3—C14—H14A	109.5
C6—C5—H5	119.2	N3—C14—H14B	109.5
C4—C5—H5	119.2	H14A—C14—H14B	109.5
C5—C6—C1	120.75 (18)	N3—C14—H14C	109.5
C5—C6—H6	119.6	H14A—C14—H14C	109.5
C1—C6—H6	119.6	H14B—C14—H14C	109.5
O2—C7—O1	122.73 (19)	C1—N1—H1A	119.5 (17)
O2—C7—C4	119.24 (19)	C1—N1—H1B	116.5 (17)
O1—C7—C4	118.02 (19)	H1A—N1—H1B	123 (2)
N2—C8—C9	122.2 (2)	C8—N2—C12	119.2 (2)
N2—C8—H8	118.9	C8—N2—H2A	117.7 (16)
C9—C8—H8	118.9	C12—N2—H2A	123.0 (16)
C8—C9—C10	120.7 (2)	C10—N3—C13	121.4 (2)
C8—C9—H9	119.7	C10—N3—C14	122.4 (2)
C10—C9—H9	119.7	C13—N3—C14	116.2 (2)
N3—C10—C11	122.6 (2)	H3A—O3—H3B	107 (4)
N3—C10—C9	121.7 (2)	H4A—O4—H4B	112 (4)
C11—C10—C9	115.7 (2)		
N1—C1—C2—C3	-177.90 (19)	C5—C4—C7—O1	-7.6 (3)
C6—C1—C2—C3	0.7 (3)	N2—C8—C9—C10	-0.3 (4)
C1—C2—C3—C4	-1.1 (3)	C8—C9—C10—N3	-178.1 (2)
C2—C3—C4—C5	0.4 (3)	C8—C9—C10—C11	0.5 (4)
C2—C3—C4—C7	-178.23 (18)	N3—C10—C11—C12	178.6 (3)
C3—C4—C5—C6	0.7 (3)	C9—C10—C11—C12	0.1 (4)
C7—C4—C5—C6	179.30 (18)	C10—C11—C12—N2	-0.8 (5)
C4—C5—C6—C1	-1.1 (3)	C9—C8—N2—C12	-0.5 (4)
N1—C1—C6—C5	178.9 (2)	C11—C12—N2—C8	1.0 (4)
C2—C1—C6—C5	0.4 (3)	C11—C10—N3—C13	-3.7 (4)
C3—C4—C7—O2	-8.6 (3)	C9—C10—N3—C13	174.7 (3)
C5—C4—C7—O2	172.8 (2)	C11—C10—N3—C14	178.0 (3)
C3—C4—C7—O1	171.01 (18)	C9—C10—N3—C14	-3.5 (4)

Hydrogen-bond geometry (\AA , $^\circ$)

Cg2 is the centroid of the C1—C6 benzene ring.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1—H1A \cdots O3 ⁱ	0.87 (1)	2.04 (1)	2.898 (3)	167 (2)
N1—H1B \cdots O4 ⁱ	0.89 (1)	2.04 (1)	2.921 (3)	174 (2)
N2—H2A \cdots O1 ⁱⁱ	0.89 (1)	1.81 (1)	2.697 (2)	174 (2)
O3—H3A \cdots O2 ⁱⁱⁱ	0.83 (1)	2.03 (1)	2.858 (3)	175 (4)
O3—H3B \cdots O1 ^{iv}	0.83 (1)	2.04 (1)	2.861 (3)	174 (4)
O4—H4A \cdots O2 ^v	0.82 (1)	2.01 (1)	2.834 (3)	175 (4)
O4—H4B \cdots O1 ^{vi}	0.82 (1)	2.04 (1)	2.847 (3)	167 (4)

C9—H9...Cg ^{2vii}	0.93	2.80	3.510 (3)	134
C12—H12...Cg ²ⁱ	0.93	2.84	3.535 (3)	132

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $x, y-1, z+1$; (iii) $-x+1, -y+2, -z$; (iv) $x+1, y, z$; (v) $x, y, z+1$; (vi) $-x+1, -y+2, -z+1$; (vii) $-x, -y+1, -z+1$.