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3-Methylpyridinium 4-nitrobenzoate–4-nitrobenzoic acid (1/1)

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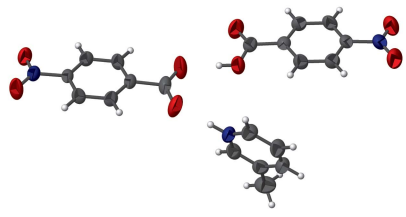
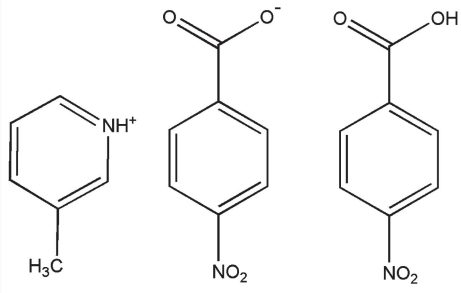
In the title compound, $C_6H_8N^+\cdot C_7H_4NO_4^-\cdot C_7H_5NO_4$, the cation is protonated at its pyridine N atom and makes a dihedral angle of 74.14 (12)° with the benzene ring of the anion. The benzene ring of the neutral molecule and the pyridine ring are inclined at an angle of 79.20 (12)°. The two benzene rings form a dihedral angle of 6.00 (12)° with each other. In the crystal, N—H···O, O—H···O and C—H···O hydrogen bonds link the cations, anions and neutral molecules to form layers parallel to the *ac* plane, which enlose $R_4^4(18)$ ring motifs. The layers are linked by further C—H···O hydrogen bonds and C—H···π interactions, forming a three-dimensional supramolecular architecture.

3D view



Chemical scheme



Structure description

Pyridine derivatives are known to exhibit pharmacological properties such as anti-inflammatory (Abdel-Alim *et al.*, 2005), anticancer (Girgis *et al.*, 2006) and anxiolytic (Spanka *et al.*, 2010) activities. We herewith report the synthesis and the crystal structure of the title compound (Fig. 1). The geometric parameters are comparable to those of reported similar structures (Quah *et al.*, 2008, 2010).

The title compound contains a 3-methylpyridinium cation protonated at its N atom, a 4-nitrobenzoate deprotonated at its hydroxy O atom and a neutral 4-nitrobenzoic acid molecule. The benzene rings (C1–C6 and C8–C13) make a dihedral angle of 6.00 (12)°. The C8–C13 benzene ring of the anion forms a dihedral angle of 74.14 (12)° with the pyridine ring (N3/C15–C19) of the cation. The C1–C6 benzene ring of the neutral molecule and the pyridine ring of the caion are inclined at an angle of 79.20 (12)°.

In the crystal, N—H···O, O—H···O and C—H···O hydrogen bonds link the cations, anions and neutral molecules to form layers parallel to (010) (Fig. 2 and Table 1), which enclose $R_4^4(18)$ ring motifs (Bernstein *et al.*, 1995). The layers are linked by further C—

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

*Cg*2 is the centroid of the ring (C1-C6)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3*A*···O4	0.88 (2)	1.73 (2)	2.612 (3)	175 (3)
O6—H6*A*···O3	0.83 (2)	1.70 (2)	2.518 (2)	175 (4)
C9—H9···O1^{i}	0.93	2.47	3.271 (3)	144
C15—H15···O3^{ii}	0.93	2.41	3.218 (3)	145
C16—H16···O2^{i}	0.93	2.59	3.353 (3)	140
C19—H19···O5^{iii}	0.93	2.42	3.293 (3)	156
C13—H13···*Cg*2^{iv}	0.93	2.83	3.564 (3)	137

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

H···O hydrogen bonds and C—H···π interactions, forming a three-dimensional structure (Fig. 2 and Table 1).

Synthesis and crystallization

The title compound was synthesized using the raw materials 4-nitrobenzoic acid (1.67 g) and 3-methylpyridine (0.93 g) in an equimolar ratio. These reactants were dissolved in 15 ml of acetone and stirred for 4 h and the solution was kept at room temperature. After a span of 10 d, single crystals suitable for X-ray diffraction were harvested.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_6H_8N^+·C_7H_4NO_4^-·C_7H_5NO_4$
M_r	427.37
Crystal system, space group	Monoclinic, $P2_1$
Temperature (K)	295
a, b, c (Å)	6.3586 (4), 13.6276 (9), 11.7469 (8)
β (°)	104.559 (2)
V (Å^3)	985.21 (11)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.11
Crystal size (mm)	0.28 × 0.24 × 0.20
Data collection	
Diffractometer	Bruker Kappa APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2004)
T_{min}, T_{max}	0.969, 0.978
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	17209, 4526, 3163
R_{int}	0.026
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.658
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.045, 0.117, 1.09
No. of reflections	4526
No. of parameters	288
No. of restraints	3
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.15, −0.19
Absolute structure	Flack (1983), 2158 Friedel pairs
Absolute structure parameter	0.3 (12)

Computer programs: *APEX2* and *SAINT* (Bruker, 2004), *SHELXS97* and *SHELXL97* (Sheldrick, 2008) and *PLATON* (Spek, 2009).

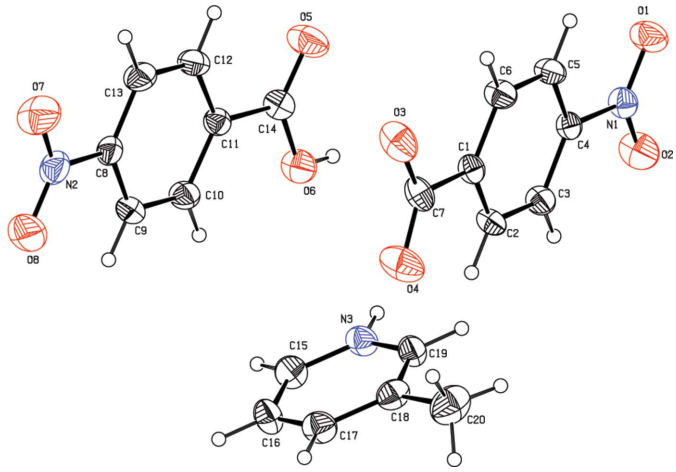


Figure 1
The molecular structure of the title molecular salt, showing the atom labelling and 30% probability displacement ellipsoids.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

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

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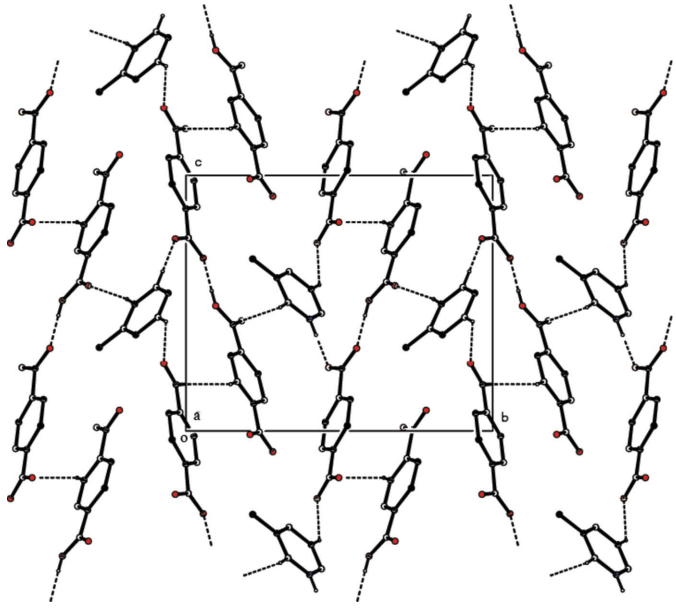

Figure 2
The crystal packing of the title compound viewed along the *a* axis. The hydrogen bonds are shown as dashed lines (see Table 1) and C-bound H atoms have been omitted for clarity.

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full crystallographic data

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Crystal data

$C_6H_8N^+·C_7H_4NO_4^-·C_7H_5NO_4$
M_r = 427.37
Monoclinic, $P2_1$
Hall symbol: P 2yb
a = 6.3586 (4) Å
b = 13.6276 (9) Å
c = 11.7469 (8) Å
β = 104.559 (2)°
V = 985.21 (11) Å^3
Z = 2
$F(000)$ = 444
D_x = 1.441 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 6874 reflections
θ = 2.3–27.7°
μ = 0.11 mm^{-1}
T = 295 K
Block, colourless
0.28 × 0.24 × 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; Bruker, 2004)
T_{min} = 0.969, T_{max} = 0.978
17209 measured reflections
4526 independent reflections
3163 reflections with $I > 2\sigma(I)$
R_{int} = 0.026
θ_{max} = 27.9°, θ_{min} = 2.3°
h = −8→8
k = −17→17
l = −15→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.117
S = 1.09
4526 reflections
288 parameters
3 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
$w = 1/[\sigma^2(F_o^2) + (0.0465P)^2 + 0.1953P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}
Absolute structure: Flack (1983), 2158 Friedel pairs
Absolute structure parameter: 0.3 (12)

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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.8161 (4)	0.49994 (17)	0.1300 (2)	0.0378 (5)
C2	0.6831 (4)	0.45484 (19)	0.0341 (2)	0.0419 (6)
H2	0.5486	0.4309	0.0386	0.050*
C3	0.7479 (4)	0.44484 (19)	−0.0690 (2)	0.0427 (5)
H3	0.6580	0.4146	−0.1344	0.051*
C4	0.9468 (4)	0.48028 (17)	−0.07302 (19)	0.0349 (5)
C5	1.0827 (4)	0.52619 (19)	0.0205 (2)	0.0449 (6)
H5	1.2168	0.5504	0.0155	0.054*
C6	1.0143 (4)	0.5356 (2)	0.1229 (2)	0.0465 (6)
H6	1.1039	0.5664	0.1878	0.056*
C7	0.7465 (4)	0.5079 (2)	0.2437 (2)	0.0470 (6)
C8	0.6962 (4)	0.72107 (17)	0.8926 (2)	0.0424 (6)
C9	0.5585 (4)	0.66743 (18)	0.8068 (2)	0.0476 (6)
H9	0.4260	0.6453	0.8170	0.057*
C10	0.6199 (4)	0.64688 (18)	0.7053 (2)	0.0457 (6)
H10	0.5279	0.6107	0.6461	0.055*
C11	0.8168 (4)	0.67933 (17)	0.6901 (2)	0.0382 (5)
C12	0.9493 (4)	0.73511 (19)	0.7767 (2)	0.0497 (6)
H12	1.0797	0.7592	0.7657	0.060*
C13	0.8912 (4)	0.7557 (2)	0.8794 (2)	0.0527 (7)
H13	0.9822	0.7924	0.9385	0.063*
C14	0.8932 (4)	0.65374 (19)	0.5837 (2)	0.0446 (6)
C15	0.2977 (4)	0.4418 (2)	0.4604 (2)	0.0528 (7)
H15	0.2215	0.4912	0.4126	0.063*
C16	0.2287 (4)	0.4086 (2)	0.5548 (3)	0.0559 (7)
H16	0.1051	0.4348	0.5719	0.067*
C17	0.3447 (4)	0.3362 (2)	0.6236 (2)	0.0543 (7)
H17	0.2990	0.3133	0.6880	0.065*
C18	0.5276 (4)	0.29665 (19)	0.5995 (2)	0.0507 (6)
C19	0.5870 (4)	0.3329 (2)	0.5033 (2)	0.0503 (6)
H19	0.7092	0.3076	0.4838	0.060*
C20	0.6584 (6)	0.2177 (2)	0.6733 (3)	0.0765 (9)
H20A	0.7627	0.1923	0.6344	0.115*
H20B	0.5636	0.1658	0.6846	0.115*
H20C	0.7328	0.2444	0.7482	0.115*

N1	1.0198 (3)	0.46793 (16)	−0.18151 (18)	0.0441 (5)
N2	0.6354 (4)	0.73877 (16)	1.0040 (2)	0.0575 (6)
N3	0.4733 (3)	0.40344 (17)	0.43743 (19)	0.0485 (5)
O1	1.1985 (3)	0.49838 (15)	−0.18295 (18)	0.0653 (6)
O2	0.8982 (3)	0.42800 (18)	−0.26438 (16)	0.0692 (6)
O3	0.8656 (3)	0.55658 (17)	0.32373 (17)	0.0701 (6)
O4	0.5771 (3)	0.4654 (2)	0.24825 (17)	0.0759 (7)
O5	1.0633 (3)	0.68184 (18)	0.56883 (18)	0.0731 (6)
O6	0.7576 (3)	0.59720 (17)	0.51037 (17)	0.0586 (5)
O7	0.7626 (4)	0.78320 (19)	1.0811 (2)	0.0873 (8)
O8	0.4619 (4)	0.70915 (19)	1.0137 (2)	0.0846 (7)
H3A	0.517 (4)	0.424 (2)	0.3758 (17)	0.067 (9)*
H6A	0.801 (6)	0.584 (3)	0.452 (2)	0.100*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0390 (12)	0.0435 (13)	0.0328 (12)	0.0039 (10)	0.0126 (10)	0.0029 (10)
C2	0.0321 (11)	0.0518 (15)	0.0440 (14)	−0.0038 (11)	0.0140 (10)	0.0000 (12)
C3	0.0387 (12)	0.0508 (14)	0.0366 (12)	−0.0029 (11)	0.0060 (10)	−0.0072 (11)
C4	0.0372 (12)	0.0384 (12)	0.0305 (12)	0.0020 (9)	0.0109 (9)	0.0006 (9)
C5	0.0374 (13)	0.0540 (16)	0.0451 (15)	−0.0107 (11)	0.0138 (11)	−0.0056 (12)
C6	0.0440 (14)	0.0603 (16)	0.0348 (13)	−0.0106 (12)	0.0095 (10)	−0.0125 (12)
C7	0.0436 (14)	0.0656 (17)	0.0348 (13)	0.0092 (12)	0.0152 (11)	0.0045 (12)
C8	0.0481 (13)	0.0364 (13)	0.0460 (14)	0.0004 (11)	0.0182 (11)	−0.0058 (11)
C9	0.0388 (13)	0.0496 (15)	0.0589 (16)	−0.0048 (11)	0.0208 (12)	−0.0046 (12)
C10	0.0404 (14)	0.0505 (15)	0.0444 (14)	−0.0067 (11)	0.0073 (11)	−0.0089 (12)
C11	0.0361 (12)	0.0393 (12)	0.0385 (13)	0.0011 (10)	0.0082 (10)	0.0019 (10)
C12	0.0420 (13)	0.0527 (16)	0.0577 (16)	−0.0122 (11)	0.0184 (12)	−0.0070 (13)
C13	0.0523 (15)	0.0526 (15)	0.0522 (16)	−0.0137 (13)	0.0113 (12)	−0.0185 (13)
C14	0.0430 (14)	0.0505 (14)	0.0399 (14)	−0.0006 (11)	0.0096 (11)	0.0036 (12)
C15	0.0530 (15)	0.0543 (16)	0.0514 (16)	0.0030 (13)	0.0138 (12)	0.0071 (13)
C16	0.0502 (15)	0.0646 (18)	0.0593 (17)	0.0085 (13)	0.0258 (13)	−0.0005 (14)
C17	0.0615 (17)	0.0599 (16)	0.0464 (15)	−0.0071 (13)	0.0230 (13)	0.0016 (13)
C18	0.0544 (16)	0.0455 (14)	0.0484 (15)	−0.0047 (12)	0.0061 (13)	−0.0015 (12)
C19	0.0424 (13)	0.0543 (15)	0.0569 (16)	0.0007 (12)	0.0177 (12)	−0.0100 (13)
C20	0.083 (2)	0.0598 (19)	0.077 (2)	0.0045 (16)	0.0011 (18)	0.0119 (17)
N1	0.0487 (12)	0.0481 (12)	0.0385 (12)	0.0018 (10)	0.0166 (10)	0.0028 (10)
N2	0.0739 (16)	0.0456 (13)	0.0613 (15)	−0.0030 (12)	0.0324 (14)	−0.0110 (12)
N3	0.0509 (12)	0.0561 (13)	0.0435 (12)	−0.0055 (10)	0.0215 (10)	0.0003 (10)
O1	0.0639 (12)	0.0816 (14)	0.0614 (13)	−0.0203 (11)	0.0363 (11)	−0.0123 (11)
O2	0.0681 (12)	0.1012 (17)	0.0398 (10)	−0.0139 (12)	0.0165 (9)	−0.0199 (11)
O3	0.0610 (12)	0.1101 (18)	0.0415 (11)	−0.0010 (12)	0.0172 (10)	−0.0187 (11)
O4	0.0703 (13)	0.1145 (19)	0.0523 (12)	−0.0193 (13)	0.0329 (10)	0.0023 (12)
O5	0.0611 (12)	0.0994 (17)	0.0672 (13)	−0.0230 (12)	0.0319 (11)	−0.0106 (12)
O6	0.0611 (12)	0.0730 (12)	0.0448 (11)	−0.0093 (10)	0.0192 (9)	−0.0126 (10)
O7	0.1097 (18)	0.0930 (18)	0.0665 (14)	−0.0288 (15)	0.0356 (13)	−0.0336 (14)
O8	0.0901 (17)	0.0946 (17)	0.0888 (17)	−0.0178 (14)	0.0592 (14)	−0.0217 (14)

Geometric parameters (Å, º)

C1—C2	1.372 (3)	C12—H12	0.9300
C1—C6	1.373 (3)	C13—H13	0.9300
C1—C7	1.514 (3)	C14—O5	1.201 (3)
C2—C3	1.381 (3)	C14—O6	1.306 (3)
C2—H2	0.9300	C15—N3	1.320 (3)
C3—C4	1.366 (3)	C15—C16	1.369 (4)
C3—H3	0.9300	C15—H15	0.9300
C4—C5	1.367 (3)	C16—C17	1.368 (4)
C4—N1	1.472 (3)	C16—H16	0.9300
C5—C6	1.383 (3)	C17—C18	1.375 (4)
C5—H5	0.9300	C17—H17	0.9300
C6—H6	0.9300	C18—C19	1.370 (4)
C7—O4	1.236 (3)	C18—C20	1.496 (4)
C7—O3	1.240 (3)	C19—N3	1.329 (4)
C8—C9	1.369 (3)	C19—H19	0.9300
C8—C13	1.372 (3)	C20—H20A	0.9600
C8—N2	1.474 (3)	C20—H20B	0.9600
C9—C10	1.374 (3)	C20—H20C	0.9600
C9—H9	0.9300	N1—O2	1.210 (3)
C10—C11	1.380 (3)	N1—O1	1.213 (2)
C10—H10	0.9300	N2—O8	1.208 (3)
C11—C12	1.375 (3)	N2—O7	1.214 (3)
C11—C14	1.492 (3)	N3—H3A	0.88 (2)
C12—C13	1.377 (4)	O6—H6A	0.82 (2)
C2—C1—C6	119.6 (2)	C8—C13—H13	120.7
C2—C1—C7	120.0 (2)	C12—C13—H13	120.7
C6—C1—C7	120.3 (2)	O5—C14—O6	124.2 (2)
C1—C2—C3	120.4 (2)	O5—C14—C11	122.8 (2)
C1—C2—H2	119.8	O6—C14—C11	113.0 (2)
C3—C2—H2	119.8	N3—C15—C16	119.6 (3)
C4—C3—C2	118.6 (2)	N3—C15—H15	120.2
C4—C3—H3	120.7	C16—C15—H15	120.2
C2—C3—H3	120.7	C17—C16—C15	118.8 (2)
C3—C4—C5	122.6 (2)	C17—C16—H16	120.6
C3—C4—N1	119.1 (2)	C15—C16—H16	120.6
C5—C4—N1	118.38 (19)	C16—C17—C18	121.3 (2)
C4—C5—C6	117.9 (2)	C16—C17—H17	119.3
C4—C5—H5	121.1	C18—C17—H17	119.3
C6—C5—H5	121.1	C19—C18—C17	116.8 (2)
C1—C6—C5	120.9 (2)	C19—C18—C20	120.6 (3)
C1—C6—H6	119.5	C17—C18—C20	122.6 (3)
C5—C6—H6	119.5	N3—C19—C18	121.2 (2)
O4—C7—O3	126.2 (2)	N3—C19—H19	119.4
O4—C7—C1	117.1 (2)	C18—C19—H19	119.4
O3—C7—C1	116.7 (2)	C18—C20—H20A	109.5

C9—C8—C13	122.0 (2)	C18—C20—H20B	109.5
C9—C8—N2	118.6 (2)	H20A—C20—H20B	109.5
C13—C8—N2	119.3 (2)	C18—C20—H20C	109.5
C8—C9—C10	118.6 (2)	H20A—C20—H20C	109.5
C8—C9—H9	120.7	H20B—C20—H20C	109.5
C10—C9—H9	120.7	O2—N1—O1	123.6 (2)
C9—C10—C11	120.8 (2)	O2—N1—C4	118.11 (19)
C9—C10—H10	119.6	O1—N1—C4	118.2 (2)
C11—C10—H10	119.6	O8—N2—O7	123.3 (2)
C12—C11—C10	119.2 (2)	O8—N2—C8	118.7 (2)
C12—C11—C14	118.7 (2)	O7—N2—C8	118.0 (2)
C10—C11—C14	122.0 (2)	C15—N3—C19	122.2 (2)
C11—C12—C13	120.7 (2)	C15—N3—H3A	119.7 (19)
C11—C12—H12	119.6	C19—N3—H3A	118.2 (19)
C13—C12—H12	119.6	C14—O6—H6A	112 (3)
C8—C13—C12	118.6 (2)		

C6—C1—C2—C3	0.2 (4)	N2—C8—C13—C12	177.4 (2)
C7—C1—C2—C3	−178.2 (2)	C11—C12—C13—C8	−1.2 (4)
C1—C2—C3—C4	0.3 (4)	C12—C11—C14—O5	−2.0 (4)
C2—C3—C4—C5	−0.8 (4)	C10—C11—C14—O5	179.5 (3)
C2—C3—C4—N1	178.5 (2)	C12—C11—C14—O6	177.2 (2)
C3—C4—C5—C6	0.7 (4)	C10—C11—C14—O6	−1.3 (3)
N1—C4—C5—C6	−178.7 (2)	N3—C15—C16—C17	0.2 (4)
C2—C1—C6—C5	−0.4 (4)	C15—C16—C17—C18	−0.1 (4)
C7—C1—C6—C5	178.1 (2)	C16—C17—C18—C19	−0.3 (4)
C4—C5—C6—C1	−0.1 (4)	C16—C17—C18—C20	179.8 (3)
C2—C1—C7—O4	5.9 (4)	C17—C18—C19—N3	0.5 (4)
C6—C1—C7—O4	−172.5 (3)	C20—C18—C19—N3	−179.5 (2)
C2—C1—C7—O3	−174.2 (2)	C3—C4—N1—O2	1.3 (3)
C6—C1—C7—O3	7.4 (4)	C5—C4—N1—O2	−179.4 (2)
C13—C8—C9—C10	0.9 (4)	C3—C4—N1—O1	−178.8 (2)
N2—C8—C9—C10	−176.9 (2)	C5—C4—N1—O1	0.6 (3)
C8—C9—C10—C11	0.2 (4)	C9—C8—N2—O8	−3.3 (4)
C9—C10—C11—C12	−1.8 (4)	C13—C8—N2—O8	178.9 (3)
C9—C10—C11—C14	176.7 (2)	C9—C8—N2—O7	177.2 (3)
C10—C11—C12—C13	2.3 (4)	C13—C8—N2—O7	−0.6 (4)
C14—C11—C12—C13	−176.2 (2)	C16—C15—N3—C19	0.0 (4)
C9—C8—C13—C12	−0.4 (4)	C18—C19—N3—C15	−0.4 (4)

Hydrogen-bond geometry (Å, º)

Cg2 is the centroid of the ring (C1-C6)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3*A*···O4	0.88 (2)	1.73 (2)	2.612 (3)	175 (3)
O6—H6*A*···O3	0.83 (2)	1.70 (2)	2.518 (2)	175 (4)
C9—H9···O1^{i}	0.93	2.47	3.271 (3)	144
C15—H15···O3^{ii}	0.93	2.41	3.218 (3)	145

C16—H16···O2^{i}	0.93	2.59	3.353 (3)	140
C19—H19···O5^{iii}	0.93	2.42	3.293 (3)	156
C13—H13···*Cg*2^{iv}	0.93	2.83	3.564 (3)	137

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