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2-Amino-5-methylpyridinium 4-chlorobenzoate

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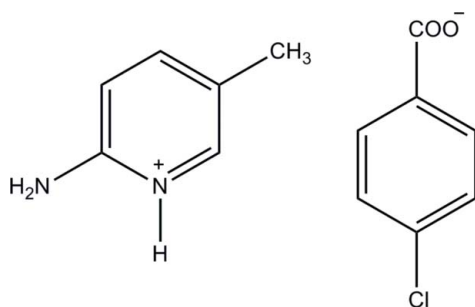
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Key indicators: single-crystal X-ray study; $T = 297$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å;
R factor = 0.047; wR factor = 0.139; data-to-parameter ratio = 26.3.

The 4-chlorobenzoate anion of the title salt, $\text{C}_6\text{H}_9\text{N}_2^+\text{C}_7\text{H}_4\text{ClO}_2^-$, is nearly planar with a dihedral angle of $5.14(16)^\circ$ between the benzene ring and the carboxylate group. In the crystal, the protonated N atom and the 2-amino group of the cation are hydrogen bonded to the carboxylate O atoms of the anion *via* a pair of $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds with an $R_2^2(8)$ ring motif. The ion pairs are further connected *via* $\text{N}-\text{H}\cdots\text{O}$ and weak $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds, forming a two-dimensional network parallel to the bc plane. The crystal structure also features a $\pi-\pi$ stacking interaction between the pyridinium and benzene rings with a centroid-centroid distance of $3.7948(9)$ Å.

Related literature

For background to the chemistry of substituted pyridines, see: Pozharski *et al.* (1997); Katritzky *et al.* (1996). For 4-chlorobenzoic acid, see: Dionysiou *et al.* (2000). For details of hydrogen-bonded supramolecular compounds, see: Aakeroy *et al.* (2002). For related structures, see: Nahrungbauer & Kvik (1977); Thanigaimani *et al.* (2012a,b,c). For hydrogen-bond motifs, see: Bernstein *et al.* (1995). For bond-length data, see: Allen *et al.* (1987).



† Thomson Reuters ResearcherID: A-5599-2009.

Experimental

Crystal data

$\text{C}_6\text{H}_9\text{N}_2^+\text{C}_7\text{H}_4\text{ClO}_2^-$
 $M_r = 264.70$
 Monoclinic, $P2_1/c$
 $a = 9.8510(6)$ Å
 $b = 10.7707(8)$ Å
 $c = 12.2123(7)$ Å
 $\beta = 102.335(2)^\circ$

$V = 1265.84(14)$ Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 0.30$ mm⁻¹
 $T = 297$ K
 $0.46 \times 0.25 \times 0.13$ mm

Data collection

Bruker SMART APEXII DUO
 CCD area-detector
 diffractometer
 Absorption correction: multi-scan
 (SADABS; Bruker, 2009)
 $T_{\min} = 0.876$, $T_{\max} = 0.963$

17572 measured reflections
 4628 independent reflections
 2976 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.034$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.047$
 $wR(F^2) = 0.139$
 $S = 1.04$
 4628 reflections
 176 parameters

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\max} = 0.30$ e Å⁻³
 $\Delta\rho_{\min} = -0.31$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N2}-\text{H1N2}\cdots\text{O1}$	0.85 (2)	2.02 (2)	2.8654 (18)	174.1 (19)
$\text{N1}-\text{H1N1}\cdots\text{O1}^i$	0.98 (2)	1.75 (2)	2.7255 (14)	174.1 (16)
$\text{N2}-\text{H2N2}\cdots\text{O2}^j$	0.92 (2)	1.83 (2)	2.7437 (17)	172.7 (18)
$\text{C2}-\text{H2A}\cdots\text{O2}^{ii}$	0.93	2.40	3.1459 (18)	137

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

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

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS5231).

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supporting information

Acta Cryst. (2013). E69, o134–o135 [https://doi.org/10.1107/S1600536812051021]

2-Amino-5-methylpyridinium 4-chlorobenzoate

Kaliyaperumal Thanigaimani, Abbas Farhadikoutenaei, Suhana Arshad and Ibrahim Abdul Razak

S1. Comment

In recent years, hydrogen bonds have attracted the interest of chemists and have been widely used to design and synthesize one, two and three-dimensional supramolecular compounds (Aakeroy *et al.*, 2002). Pyridine and its derivatives play an important role in heterocyclic chemistry (Pozharski *et al.*, 1997; Katritzky *et al.*, 1996). They are often involved in hydrogen-bond interactions. 4-Chlorobenzoic acid (4-CBA) has been reported as intermediate product during biological or chemical degradation of pesticides and herbicides (Dionysiou *et al.*, 2000). We have recently reported related crystal structures of 2-amino-5-methylpyridinium 3-chlorobenzoate (Thanigaimani *et al.*, 2012*a*), 2-amino-5-methylpyridinium 2-aminobenzoate (Thanigaimani *et al.*, 2012*b*) and 2-amino-5-methylpyridinium trifluoroacetate (Thanigaimani *et al.*, 2012*c*). In order to study some interesting hydrogen bonding interactions of this compound, the synthesis and structure of the title salt is presented here.

The asymmetric unit (Fig. 1) contains one 2-amino-5-methylpyridinium cation and one 4-chlorobenzoate anion. The proton transfers from the carboxyl group oxygen atom (O1) to atom N1 of the 2-amino-5-methylpyrimidine resulted in the widening of C1—N1—C5 angle of the pyridinium ring to 122.06 (11)°, compared to the corresponding angle of 117.4 (3)° in neutral 2-amino-5-methylpyridine (Nahringbauer & Kvik, 1977). The 2-amino-5-methylpyridinium cation is essentially planar, with a maximum deviation of 0.005 (1) Å for atom C1. The carboxylate group of the 4-chlorobenzoate anion is slightly twisted from the attached ring with the dihedral angle between C7—C12 ring and O1/O2/C13 plane being 5.14 (16)°. The bond lengths (Allen *et al.*, 1987) and angles are normal.

In the crystal packing (Fig. 2), the protonated N1 atom and a nitrogen atom of the 2-amino group (N2) are hydrogen-bonded to the carboxylate oxygen atoms (O1 and O2) *via* a pair of intermolecular N1—H1N1ⁱ⋯O1ⁱ and N2—H2N2ⁱⁱ⋯O2ⁱⁱ hydrogen bonds (symmetry code in Table 1), forming a ring motif of $R_2^2(8)$ (Bernstein *et al.*, 1995). Furthermore, these motifs are connected *via* N2—H1N2ⁱ⋯O1 and C2—H2Aⁱⁱ⋯O2ⁱⁱ hydrogen bonds to form a two-dimensional network parallel to the *bc* plane. The crystal structure is further stabilized by π – π interactions between the pyridine (C1–C5/N1) and benzene (C7–C12) rings, with centroid to centroid distance of 3.7948 (9) Å (symmetry codes: 1 - *x*, -1/2 + *y*, 1/2 - *z* and 1 - *x*, 1/2 + *y*, 1/2 - *z*)

S2. Experimental

Hot methanol solutions (20 ml) of 2-amino-5-methylpyridine (54 mg, Aldrich) and 4-chlorobenzoic acid (39 mg, Aldrich) were mixed and warmed over a heating magnetic stirrer hotplate for a few minutes. The resulting solution was allowed to cool slowly at room temperature and crystals of the title compound (I) appeared after a few days.

S3. Refinement

N-bound H atoms were located in a difference Fourier maps and refined freely [refined N—H distances 0.98 (2), 0.92 (2) and 0.85 (2) Å]. The remaining H atoms were positioned geometrically (C—H = 0.93–0.96 Å) and were refined using a

riding model, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ or $1.5U_{\text{eq}}(\text{methyl C})$. A rotating group model was used for the methyl group. Three outliers were omitted (1 4 0, 1 1 0 and 3 1 2) in the final refinement.

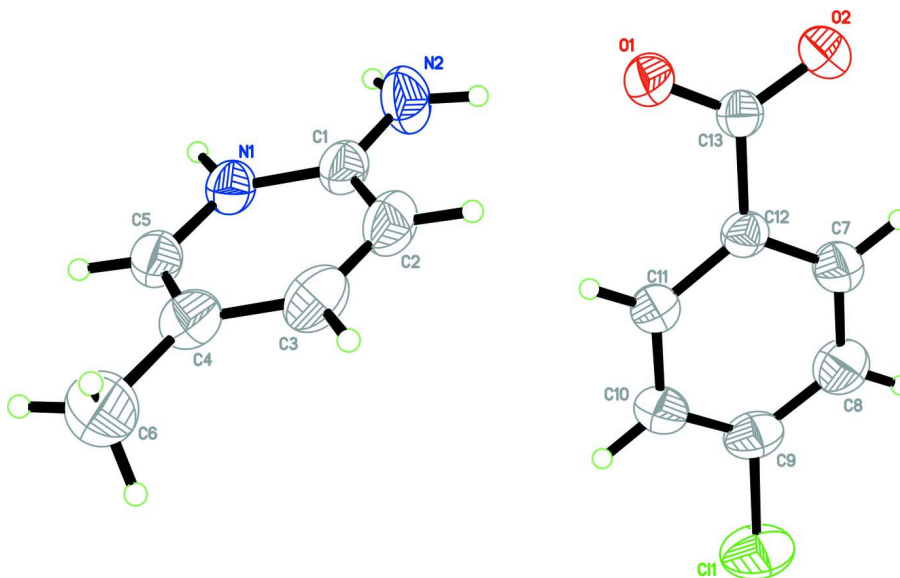


Figure 1

The molecular structure of the title compound with atom labels with 50% probability displacement ellipsoids.

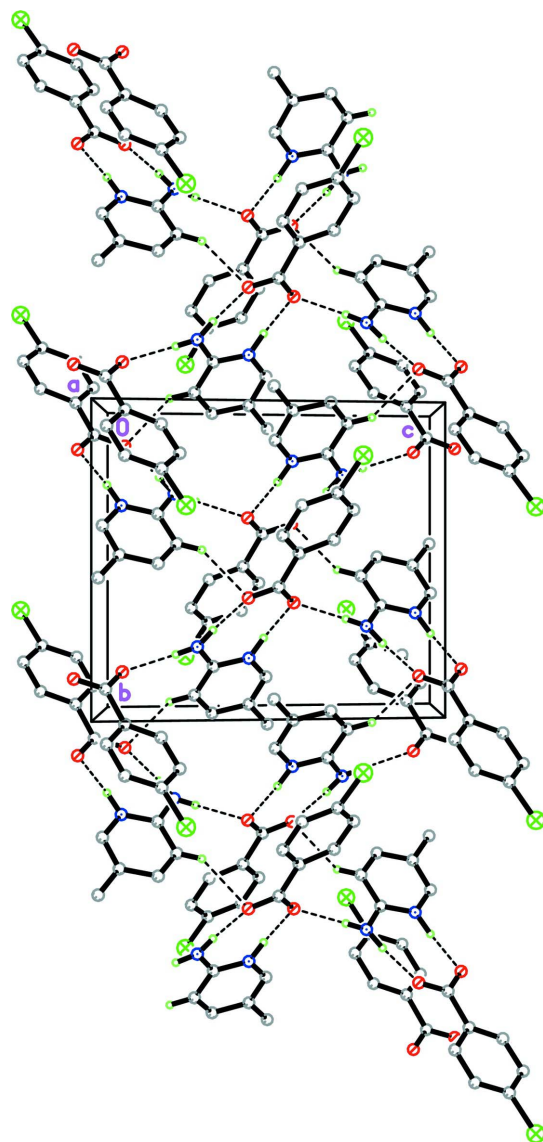


Figure 2

The crystal packing of the title compound. The H atoms not involved in the intermolecular interactions (dashed lines) have been omitted for clarity.

2-Amino-5-methylpyridinium 4-chlorobenzoate

Crystal data

$C_6H_9N_2^+ \cdot C_7H_4ClO_2^-$

$M_r = 264.70$

Monoclinic, $P2_1/c$

Hall symbol: $-P\ 2_1/c$

$a = 9.8510$ (6) Å

$b = 10.7707$ (8) Å

$c = 12.2123$ (7) Å

$\beta = 102.335$ (2)°

$V = 1265.84$ (14) Å³

$Z = 4$

$F(000) = 552$

$D_x = 1.389$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 3497 reflections

$\theta = 2.6$ – 26.9 °

$\mu = 0.30$ mm⁻¹

$T = 297$ K

Plate, colourless

$0.46 \times 0.25 \times 0.13$ mm

Data collection

Bruker SMART APEXII DUO CCD area-detector
 diffractometer
 Radiation source: fine-focus sealed tube
 Graphite monochromator
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Bruker, 2009)
 $T_{\min} = 0.876$, $T_{\max} = 0.963$

17572 measured reflections
 4628 independent reflections
 2976 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.034$
 $\theta_{\max} = 32.8^\circ$, $\theta_{\min} = 2.6^\circ$
 $h = -14 \rightarrow 15$
 $k = -16 \rightarrow 16$
 $l = -18 \rightarrow 17$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.047$
 $wR(F^2) = 0.139$
 $S = 1.04$
 4628 reflections
 176 parameters
 0 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
 $w = 1/[\sigma^2(F_o^2) + (0.0608P)^2 + 0.1513P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.30 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.31 \text{ e } \text{\AA}^{-3}$

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C11	-0.02173 (5)	0.82984 (4)	0.23669 (4)	0.07093 (17)
O1	0.41482 (11)	0.36071 (10)	0.43150 (8)	0.0468 (2)
O2	0.29316 (12)	0.37788 (10)	0.56405 (8)	0.0521 (3)
N1	0.54982 (12)	0.32374 (10)	0.06443 (9)	0.0384 (2)
N2	0.44920 (16)	0.28252 (14)	0.21480 (12)	0.0534 (3)
C1	0.53584 (14)	0.34947 (12)	0.16960 (11)	0.0393 (3)
C2	0.61705 (15)	0.44688 (14)	0.22692 (12)	0.0462 (3)
H2A	0.6104	0.4672	0.2996	0.055*
C3	0.70468 (15)	0.51067 (14)	0.17600 (13)	0.0490 (3)
H3A	0.7581	0.5743	0.2148	0.059*
C4	0.71723 (14)	0.48309 (13)	0.06545 (12)	0.0452 (3)
C5	0.63774 (14)	0.38868 (13)	0.01390 (11)	0.0416 (3)
H5A	0.6435	0.3675	-0.0588	0.050*
C6	0.81460 (18)	0.55543 (18)	0.01020 (17)	0.0643 (4)
H6A	0.8137	0.5209	-0.0624	0.096*

H6B	0.9070	0.5510	0.0555	0.096*
H6C	0.7853	0.6406	0.0022	0.096*
C7	0.14475 (15)	0.57790 (14)	0.46421 (12)	0.0449 (3)
H7A	0.1323	0.5510	0.5338	0.054*
C8	0.06266 (16)	0.67279 (15)	0.40995 (14)	0.0530 (4)
H8A	-0.0053	0.7091	0.4420	0.064*
C9	0.08322 (14)	0.71276 (13)	0.30744 (12)	0.0452 (3)
C10	0.18420 (16)	0.66134 (13)	0.25949 (12)	0.0452 (3)
H10A	0.1978	0.6902	0.1909	0.054*
C11	0.26556 (14)	0.56587 (12)	0.31472 (11)	0.0399 (3)
H11A	0.3344	0.5309	0.2830	0.048*
C12	0.24526 (12)	0.52207 (11)	0.41692 (10)	0.0336 (2)
C13	0.32454 (13)	0.41235 (11)	0.47546 (10)	0.0356 (3)
H1N1	0.4981 (19)	0.2561 (18)	0.0206 (15)	0.067 (5)*
H2N2	0.393 (2)	0.227 (2)	0.1687 (17)	0.075 (6)*
H1N2	0.4328 (19)	0.3062 (17)	0.2770 (17)	0.060 (5)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C11	0.0665 (3)	0.0571 (3)	0.0817 (3)	0.02362 (19)	-0.0011 (2)	0.0172 (2)
O1	0.0589 (6)	0.0468 (5)	0.0353 (5)	0.0185 (4)	0.0114 (4)	0.0030 (4)
O2	0.0713 (7)	0.0503 (6)	0.0373 (5)	0.0150 (5)	0.0171 (5)	0.0093 (4)
N1	0.0453 (6)	0.0363 (5)	0.0330 (5)	0.0000 (4)	0.0069 (4)	-0.0063 (4)
N2	0.0695 (8)	0.0554 (8)	0.0388 (6)	-0.0138 (7)	0.0196 (6)	-0.0123 (6)
C1	0.0468 (7)	0.0369 (6)	0.0332 (6)	0.0043 (5)	0.0063 (5)	-0.0056 (5)
C2	0.0529 (8)	0.0457 (7)	0.0384 (7)	0.0010 (6)	0.0060 (6)	-0.0134 (6)
C3	0.0460 (7)	0.0418 (7)	0.0564 (8)	-0.0020 (6)	0.0050 (6)	-0.0140 (6)
C4	0.0424 (7)	0.0400 (7)	0.0532 (8)	0.0028 (5)	0.0102 (6)	-0.0018 (6)
C5	0.0457 (7)	0.0415 (7)	0.0380 (6)	0.0048 (5)	0.0101 (5)	-0.0026 (5)
C6	0.0588 (9)	0.0611 (10)	0.0768 (12)	-0.0101 (8)	0.0231 (8)	-0.0026 (9)
C7	0.0498 (7)	0.0446 (7)	0.0428 (7)	0.0064 (6)	0.0157 (6)	0.0043 (6)
C8	0.0503 (8)	0.0513 (8)	0.0608 (9)	0.0148 (6)	0.0195 (7)	0.0036 (7)
C9	0.0414 (7)	0.0365 (6)	0.0533 (8)	0.0052 (5)	-0.0001 (6)	0.0030 (6)
C10	0.0534 (8)	0.0405 (7)	0.0408 (7)	0.0040 (6)	0.0083 (6)	0.0073 (5)
C11	0.0442 (6)	0.0379 (6)	0.0389 (6)	0.0053 (5)	0.0117 (5)	0.0023 (5)
C12	0.0365 (6)	0.0295 (5)	0.0330 (6)	-0.0017 (4)	0.0036 (4)	-0.0022 (4)
C13	0.0453 (6)	0.0314 (6)	0.0280 (5)	0.0013 (5)	0.0029 (5)	-0.0029 (4)

Geometric parameters (Å, °)

C11—C9	1.7390 (14)	C5—H5A	0.9300
O1—C13	1.2619 (16)	C6—H6A	0.9600
O2—C13	1.2436 (16)	C6—H6B	0.9600
N1—C1	1.3495 (16)	C6—H6C	0.9600
N1—C5	1.3596 (18)	C7—C8	1.382 (2)
N1—H1N1	0.98 (2)	C7—C12	1.3856 (18)
N2—C1	1.3245 (19)	C7—H7A	0.9300

N2—H2N2	0.92 (2)	C8—C9	1.379 (2)
N2—H1N2	0.85 (2)	C8—H8A	0.9300
C1—C2	1.4113 (19)	C9—C10	1.374 (2)
C2—C3	1.354 (2)	C10—C11	1.3870 (18)
C2—H2A	0.9300	C10—H10A	0.9300
C3—C4	1.413 (2)	C11—C12	1.3881 (18)
C3—H3A	0.9300	C11—H11A	0.9300
C4—C5	1.3539 (19)	C12—C13	1.5097 (16)
C4—C6	1.503 (2)		
C1—N1—C5	122.05 (12)	C4—C6—H6C	109.5
C1—N1—H1N1	121.7 (10)	H6A—C6—H6C	109.5
C5—N1—H1N1	116.2 (10)	H6B—C6—H6C	109.5
C1—N2—H2N2	117.2 (12)	C8—C7—C12	121.22 (13)
C1—N2—H1N2	118.2 (13)	C8—C7—H7A	119.4
H2N2—N2—H1N2	122.3 (17)	C12—C7—H7A	119.4
N2—C1—N1	119.39 (13)	C9—C8—C7	118.80 (13)
N2—C1—C2	123.06 (13)	C9—C8—H8A	120.6
N1—C1—C2	117.55 (13)	C7—C8—H8A	120.6
C3—C2—C1	119.92 (13)	C10—C9—C8	121.41 (13)
C3—C2—H2A	120.0	C10—C9—C11	119.23 (12)
C1—C2—H2A	120.0	C8—C9—C11	119.36 (11)
C2—C3—C4	121.78 (13)	C9—C10—C11	119.16 (13)
C2—C3—H3A	119.1	C9—C10—H10A	120.4
C4—C3—H3A	119.1	C11—C10—H10A	120.4
C5—C4—C3	116.24 (13)	C10—C11—C12	120.66 (12)
C5—C4—C6	122.81 (14)	C10—C11—H11A	119.7
C3—C4—C6	120.95 (14)	C12—C11—H11A	119.7
C4—C5—N1	122.46 (13)	C7—C12—C11	118.71 (12)
C4—C5—H5A	118.8	C7—C12—C13	119.06 (11)
N1—C5—H5A	118.8	C11—C12—C13	122.18 (11)
C4—C6—H6A	109.5	O2—C13—O1	124.56 (12)
C4—C6—H6B	109.5	O2—C13—C12	116.49 (11)
H6A—C6—H6B	109.5	O1—C13—C12	118.93 (11)
C5—N1—C1—N2	-179.57 (13)	C7—C8—C9—C11	178.64 (12)
C5—N1—C1—C2	-0.37 (19)	C8—C9—C10—C11	1.0 (2)
N2—C1—C2—C3	179.28 (15)	C11—C9—C10—C11	-178.43 (11)
N1—C1—C2—C3	0.1 (2)	C9—C10—C11—C12	0.3 (2)
C1—C2—C3—C4	0.4 (2)	C8—C7—C12—C11	2.0 (2)
C2—C3—C4—C5	-0.6 (2)	C8—C7—C12—C13	-175.35 (13)
C2—C3—C4—C6	179.69 (15)	C10—C11—C12—C7	-1.8 (2)
C3—C4—C5—N1	0.3 (2)	C10—C11—C12—C13	175.48 (12)
C6—C4—C5—N1	-179.95 (14)	C7—C12—C13—O2	0.45 (17)
C1—N1—C5—C4	0.1 (2)	C11—C12—C13—O2	-176.81 (12)
C12—C7—C8—C9	-0.7 (2)	C7—C12—C13—O1	179.13 (12)
C7—C8—C9—C10	-0.8 (2)	C11—C12—C13—O1	1.87 (18)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
N2—H1N2 \cdots O1	0.85 (2)	2.02 (2)	2.8654 (18)	174.1 (19)
N1—H1N1 \cdots O1 ⁱ	0.98 (2)	1.75 (2)	2.7255 (14)	174.1 (16)
N2—H2N2 \cdots O2 ⁱ	0.92 (2)	1.83 (2)	2.7437 (17)	172.7 (18)
C2—H2A \cdots O2 ⁱⁱ	0.93	2.40	3.1459 (18)	137

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