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4-Chloroanilinium 2-carboxy-4,5-dichlorobenzoate

 Graham Smith,^{a*} Urs D. Wermuth^a and Jonathan M. White^b
^aSchool of Physical and Chemical Sciences, Queensland University of Technology, GPO Box 2434, Brisbane, Queensland 4001, Australia, and ^bBIO-21 Molecular Science and Biotechnology, University of Melbourne, Parkville, Victoria 3052, Australia

Correspondence e-mail: g.smith@qut.edu.au

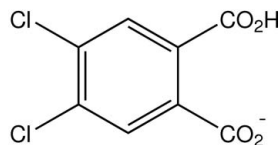
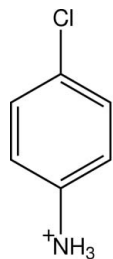
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 Key indicators: single-crystal X-ray study; $T = 130$ K; mean $\sigma(\text{C}-\text{C}) = 0.009$ Å; R factor = 0.062; wR factor = 0.175; data-to-parameter ratio = 10.6.

The structure of the 1:1 proton-transfer compound of 4-chloroaniline with 4,5-dichlorophthalic acid (DCPA), *viz.* $\text{C}_6\text{H}_7\text{ClN}^+\cdot\text{C}_8\text{H}_3\text{Cl}_2\text{O}_4^-$, has been determined at 130 K. The non-planar hydrogen phthalate anions and the 4-chloroanilinium cations form two-dimensional $\text{O}-\text{H}\cdots\text{O}$ and $\text{N}-\text{H}\cdots\text{O}$ hydrogen-bonded substructures which have no peripheral extension. Between the sheets there are weak $\pi-\pi$ associations between alternating cation-anion aromatic ring systems [shortest centroid-centroid separation = 3.735 (4) Å].

Related literature

For the structures of other hydrogen DCPA salts with aromatic Lewis bases showing similar two-dimensional substructures, see: Smith *et al.* (2008*b*). This contrasts with the majority of the compounds in which the DCPA anion is planar with a short intramolecular carboxylic acid hydrogen bond, see: Smith *et al.* (2007, 2008*a*, 2009).



Experimental

Crystal data

 $\text{C}_6\text{H}_7\text{ClN}^+\cdot\text{C}_8\text{H}_3\text{Cl}_2\text{O}_4^-$
 $M_r = 362.58$
 Monoclinic, $C2$
 $a = 12.8171$ (8) Å
 $b = 7.5954$ (3) Å
 $c = 16.0909$ (6) Å

 $\beta = 109.815$ (5)°
 $V = 1473.72$ (13) Å³
 $Z = 4$
 Cu $K\alpha$ radiation

 $\mu = 5.80$ mm⁻¹
 $T = 130$ K
 $0.34 \times 0.27 \times 0.05$ mm

Data collection

 Oxford Diffraction Gemini Ultra
 CCD-detector diffractometer
 Absorption correction: multi-scan
 (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.201$, $T_{\max} = 0.748$

 3680 measured reflections
 2288 independent reflections
 1879 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.061$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.062$
 $wR(F^2) = 0.175$
 $S = 1.00$
 2288 reflections
 215 parameters
 1 restraint

 H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\text{max}} = 0.64$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.56$ e Å⁻³
 Absolute structure: Flack (1983), 723 Friedel pairs
 Flack parameter: 0.04 (3)

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{O12}-\text{H12}\cdots\text{O21}^{\text{i}}$	0.81 (3)	1.69 (3)	2.485 (5)	166 (4)
$\text{N1A}-\text{H11A}\cdots\text{O11}^{\text{ii}}$	0.89 (4)	2.03 (4)	2.867 (8)	157 (4)
$\text{N1A}-\text{H11A}\cdots\text{O22}$	0.89 (4)	2.59 (4)	2.875 (7)	100 (2)
$\text{N1A}-\text{H12A}\cdots\text{O22}$	0.88 (3)	2.58 (5)	2.875 (7)	100 (3)
$\text{N1A}-\text{H12A}\cdots\text{O22}^{\text{iii}}$	0.88 (3)	1.94 (3)	2.813 (6)	172 (5)
$\text{N1A}-\text{H13A}\cdots\text{O12}^{\text{iv}}$	0.88 (4)	2.58 (5)	3.019 (7)	112 (3)
$\text{N1A}-\text{H13A}\cdots\text{O21}^{\text{iv}}$	0.88 (4)	1.94 (4)	2.805 (7)	166 (4)

 Symmetry codes: (i) $-x + \frac{3}{2}, y - \frac{1}{2}, -z + 2$; (ii) $x, y + 1, z$; (iii) $-x + 1, y, -z + 2$; (iv) $x - \frac{1}{2}, y + \frac{1}{2}, z$.

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2007); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2007); data reduction: *CrysAlis RED*; 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: *PLATON*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2844).

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supporting information

Acta Cryst. (2009). E65, o2111 [doi:10.1107/S160053680903044X]

4-Chloroanilinium 2-carboxy-4,5-dichlorobenzoate

Graham Smith, Urs D. Wermuth and Jonathan M. White

S1. Comment

Among the known structures of the 1:1 aromatic Lewis base compounds of 4,5-dichlorophthalic acid (DCPA), a small number have similar hydrogen-bonded substructures in which the basic $N^+—H\cdots O_{\text{carboxyl}}$ linked cation–anion unit is propagated in two dimensions (Smith *et al.*, 2008*b*). In these the DCPA anions are non-planar with the carboxylic acid and carboxylate groups rotated out of the plane of the benzene ring. This contrasts with the majority of the compounds in which the DCPA anion is planar with a short intramolecular carboxylic acid $O—H\cdots O_{\text{carboxyl}}$ hydrogen bond (Smith *et al.*, 2007, 2008*a*, 2009). Since the examples having the two-dimensional substructures were substituted anilines, the 4-chloro-analogue was reacted with DCPA, giving anhydrous 4-chloroanilinium 2-carboxy-4,5-dichlorobenzoate $C_6H_7ClN^+C_8H_3Cl_2O_4^-$ (I) and its structure is reported here.

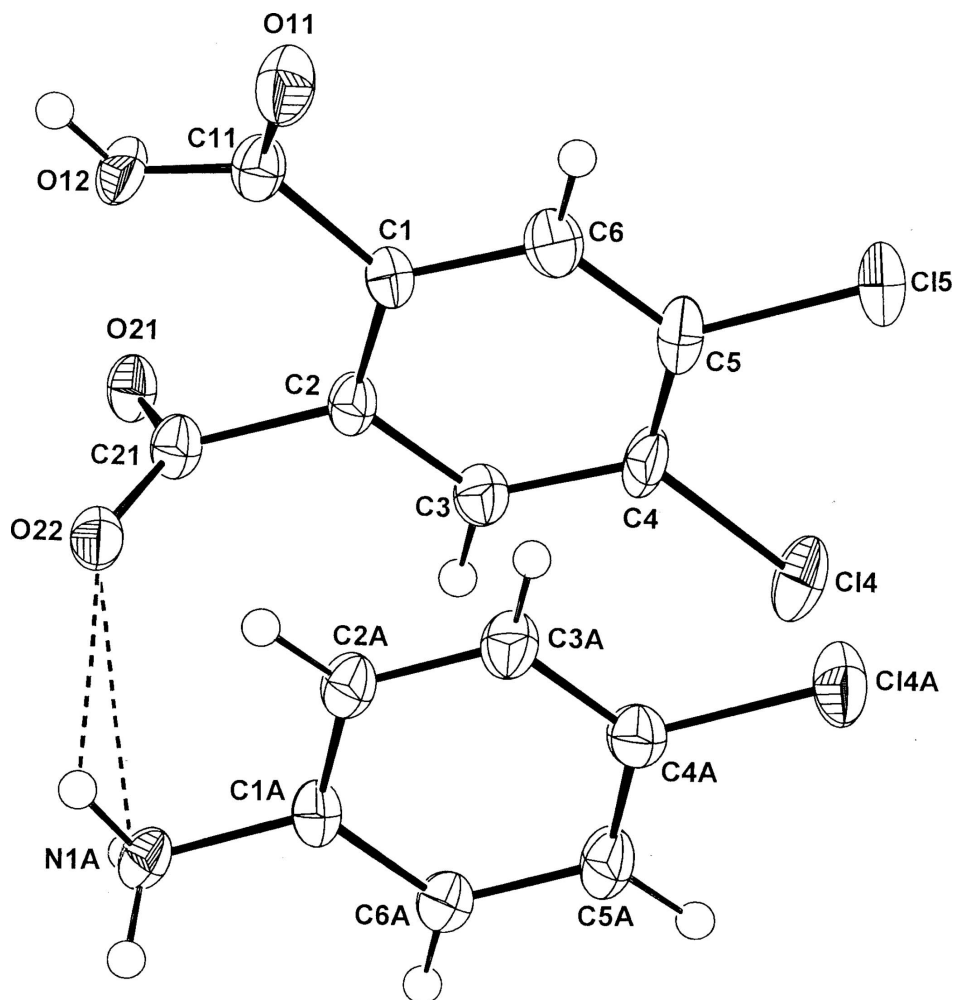
In (I), as expected, the primary hydrogen-bonded cation–anion structural unit (Fig. 1) provides the basis for formation of the previously described two-dimensional substructure which extends across the *ab* plane in the unit cell, having no lateral interactions (Fig. 2). The hydrogen bonding within the plane (Table 1) includes a cyclic $R^2_1(6)$ anilinium– $H\cdots O12, O21$ interaction. The alternating cation–anion aromatic ring systems (C1–C6 and C1A–C6A) give weak π – π interactions [shortest centroid separation 3.735 (4) Å]. The hydrogen 4,5-dichlorophthalate anion is non-planar [torsion angles C2–C1–C11–O11, 163.7 (7)°; C1–C2–C21–O22, -83.3 (8)°],

S2. Experimental

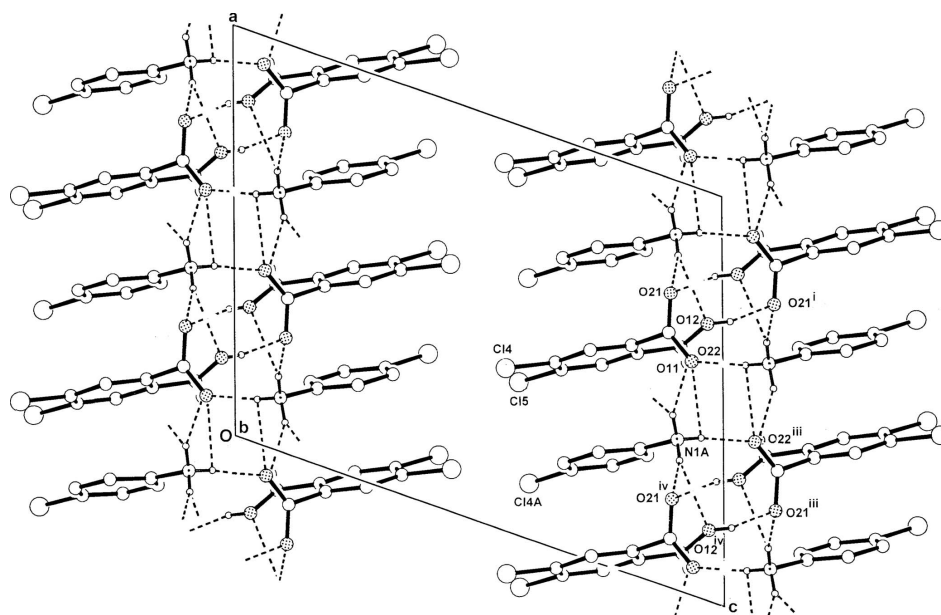
The title compound (I) was synthesized by heating together 1 mmol quantities of 4-chloroaniline and 4,5-dichlorophthalic acid in 50 ml of 50% aqueous methanol for 10 min under reflux. After concentration to *ca.* 30 ml, partial room-temperature evaporation of the hot-filtered solution gave small colourless plates [m.p. 492 K].

S3. Refinement

Hydrogen atoms potentially involved in hydrogen-bonding interactions were located by difference methods and their positional and isotropic displacement parameters were refined. Other H atoms were included in the refinement at calculated positions [C–H, 0.93 Å] and treated as riding models with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

**Figure 1**

Molecular configuration and atom numbering scheme for the 4-chloroanilinium cation and the hydrogen 4,5-dichlorophthalate anion in (I). Non-H atoms are shown as 50% probability displacement ellipsoids. Hydrogen bonds are shown as dashed lines.

**Figure 2**

The two-dimensional sheet structure in (I) viewed down the *b* axis in the unit cell. Non-interactive H atoms are omitted and hydrogen bonds are shown as dashed lines. (For symmetry codes, see Table 1).

4-Chloroanilinium 2-carboxy-4,5-dichlorobenzoate

Crystal data

$C_6H_7ClN^+ \cdot C_8H_3Cl_2O_4^-$

$M_r = 362.58$

Monoclinic, *C2*

Hall symbol: *C 2y*

$a = 12.8171 (8) \text{ \AA}$

$b = 7.5954 (3) \text{ \AA}$

$c = 16.0909 (6) \text{ \AA}$

$\beta = 109.815 (5)^\circ$

$V = 1473.72 (13) \text{ \AA}^3$

$Z = 4$

$F(000) = 736$

$D_x = 1.634 \text{ Mg m}^{-3}$

Melting point: 492 K

Cu *K* α radiation, $\lambda = 1.54184 \text{ \AA}$

Cell parameters from 1721 reflections

$\theta = 2.9\text{--}71.8^\circ$

$\mu = 5.80 \text{ mm}^{-1}$

$T = 130 \text{ K}$

Plate, colourless

$0.34 \times 0.27 \times 0.05 \text{ mm}$

Data collection

Oxford Diffraction Gemini Ultra CCD-detector diffractometer

Radiation source: Enhance Ultra (Cu) X-ray source

Mirror monochromator

ω scans

Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)

$T_{\min} = 0.201$, $T_{\max} = 0.748$

3680 measured reflections

2288 independent reflections

1879 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.061$

$\theta_{\max} = 72.1^\circ$, $\theta_{\min} = 2.9^\circ$

$h = -15 \rightarrow 14$

$k = -9 \rightarrow 8$

$l = -15 \rightarrow 19$

*Refinement*Refinement on F^2

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.062$ $wR(F^2) = 0.175$ $S = 1.00$

2288 reflections

215 parameters

1 restraint

Primary atom site location: structure-invariant
direct methodsSecondary atom site location: difference Fourier
mapHydrogen site location: inferred from
neighbouring sitesH atoms treated by a mixture of independent
and constrained refinement $w = 1/[\sigma^2(F_o^2) + (0.135P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\max} < 0.001$ $\Delta\rho_{\max} = 0.64 \text{ e } \text{\AA}^{-3}$ $\Delta\rho_{\min} = -0.56 \text{ e } \text{\AA}^{-3}$ Absolute structure: Flack (1983), 723 Friedel
pairs

Absolute structure parameter: 0.04 (3)

*Special details***Geometry.** Bond distances, angles *etc.* have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles**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)*

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Cl4	0.39571 (14)	0.8094 (3)	0.55613 (9)	0.0377 (5)
Cl5	0.37318 (14)	0.3980 (3)	0.58289 (9)	0.0418 (5)
O11	0.5642 (4)	0.3295 (7)	0.9286 (3)	0.0348 (14)
O12	0.6750 (3)	0.5632 (6)	0.9688 (2)	0.0282 (11)
O21	0.7198 (3)	0.9010 (6)	0.8943 (2)	0.0243 (10)
O22	0.5704 (3)	0.9285 (6)	0.9364 (2)	0.0272 (13)
C1	0.5441 (5)	0.5652 (8)	0.8257 (4)	0.0244 (16)
C2	0.5583 (5)	0.7457 (8)	0.8141 (3)	0.0222 (16)
C3	0.5118 (5)	0.8181 (9)	0.7299 (4)	0.0257 (16)
C4	0.4522 (5)	0.7126 (9)	0.6581 (4)	0.0289 (18)
C5	0.4402 (5)	0.5333 (9)	0.6707 (4)	0.0311 (18)
C6	0.4861 (5)	0.4599 (9)	0.7537 (4)	0.0276 (17)
C11	0.5956 (5)	0.4739 (9)	0.9139 (4)	0.0244 (17)
C21	0.6212 (4)	0.8673 (7)	0.8897 (3)	0.0237 (16)
Cl4A	0.13666 (14)	0.6564 (2)	0.60330 (9)	0.0387 (5)
N1A	0.3688 (4)	1.1240 (7)	0.9059 (3)	0.0234 (14)
C1A	0.3149 (5)	1.0096 (8)	0.8304 (3)	0.0233 (16)
C2A	0.2717 (5)	1.0813 (9)	0.7460 (4)	0.0292 (17)
C3A	0.2162 (5)	0.9729 (9)	0.6753 (4)	0.0300 (18)
C4A	0.2064 (5)	0.7965 (9)	0.6903 (4)	0.0286 (17)
C5A	0.2510 (5)	0.7210 (9)	0.7743 (4)	0.0283 (17)
C6A	0.3054 (5)	0.8316 (9)	0.8443 (3)	0.0263 (18)
H3	0.52050	0.93760	0.72140	0.0310*
H6	0.47830	0.34000	0.76170	0.0340*

H12	0.700 (3)	0.509 (4)	1.015 (2)	0.042 (11)*
H2A	0.27990	1.20080	0.73710	0.0340*
H3A	0.18610	1.01900	0.61860	0.0360*
H5A	0.24450	0.60100	0.78290	0.0340*
H6A	0.33560	0.78560	0.90100	0.0320*
H11A	0.425 (3)	1.179 (4)	0.897 (3)	0.035 (10)*
H12A	0.393 (4)	1.059 (3)	0.954 (2)	0.041 (11)*
H13A	0.320 (4)	1.202 (4)	0.910 (3)	0.038 (11)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C14	0.0444 (9)	0.0546 (10)	0.0141 (6)	-0.0005 (8)	0.0035 (5)	0.0056 (6)
C15	0.0482 (10)	0.0479 (10)	0.0206 (6)	-0.0014 (8)	0.0002 (6)	-0.0120 (6)
O11	0.038 (2)	0.035 (3)	0.026 (2)	-0.011 (2)	0.0037 (17)	0.0002 (19)
O12	0.031 (2)	0.034 (2)	0.0147 (17)	0.0000 (18)	0.0015 (15)	0.0039 (16)
O21	0.0266 (18)	0.031 (2)	0.0155 (15)	-0.0022 (18)	0.0075 (14)	-0.0015 (15)
O22	0.026 (2)	0.033 (3)	0.0203 (17)	0.0019 (17)	0.0050 (15)	-0.0038 (16)
C1	0.028 (3)	0.027 (3)	0.017 (2)	0.001 (2)	0.006 (2)	-0.004 (2)
C2	0.023 (3)	0.029 (3)	0.015 (2)	-0.001 (2)	0.007 (2)	-0.001 (2)
C3	0.028 (3)	0.029 (3)	0.020 (2)	0.001 (3)	0.008 (2)	-0.001 (2)
C4	0.029 (3)	0.043 (4)	0.011 (2)	0.002 (3)	0.002 (2)	0.000 (2)
C5	0.030 (3)	0.041 (4)	0.017 (2)	-0.005 (3)	0.001 (2)	-0.006 (3)
C6	0.030 (3)	0.031 (3)	0.024 (3)	-0.003 (3)	0.012 (2)	-0.002 (2)
C11	0.022 (3)	0.033 (3)	0.019 (3)	-0.003 (2)	0.008 (2)	-0.001 (2)
C21	0.023 (3)	0.030 (3)	0.018 (2)	-0.002 (2)	0.007 (2)	-0.001 (2)
C14A	0.0489 (9)	0.0436 (10)	0.0201 (6)	-0.0072 (8)	0.0073 (6)	-0.0054 (6)
N1A	0.023 (2)	0.030 (3)	0.016 (2)	0.001 (2)	0.0050 (16)	0.0040 (19)
C1A	0.024 (3)	0.029 (3)	0.017 (2)	-0.004 (2)	0.007 (2)	-0.003 (2)
C2A	0.036 (3)	0.029 (3)	0.020 (3)	0.005 (3)	0.006 (2)	0.001 (2)
C3A	0.034 (3)	0.039 (4)	0.016 (2)	0.000 (3)	0.007 (2)	0.001 (2)
C4A	0.035 (3)	0.029 (3)	0.022 (3)	0.003 (3)	0.010 (2)	0.000 (2)
C5A	0.032 (3)	0.031 (3)	0.021 (3)	-0.002 (3)	0.008 (2)	0.002 (2)
C6A	0.029 (3)	0.032 (4)	0.018 (2)	0.000 (3)	0.008 (2)	0.002 (2)

Geometric parameters (Å, °)

C14—C4	1.718 (6)	C2—C3	1.395 (8)
C15—C5	1.723 (7)	C3—C4	1.401 (9)
C14A—C4A	1.744 (7)	C4—C5	1.393 (10)
O11—C11	1.219 (9)	C5—C6	1.381 (9)
O12—C11	1.291 (8)	C3—H3	0.9300
O21—C21	1.267 (7)	C6—H6	0.9300
O22—C21	1.240 (6)	C1A—C6A	1.383 (9)
O12—H12	0.81 (3)	C1A—C2A	1.392 (8)
N1A—C1A	1.463 (7)	C2A—C3A	1.389 (9)
N1A—H13A	0.89 (4)	C3A—C4A	1.375 (10)
N1A—H12A	0.88 (3)	C4A—C5A	1.400 (9)

N1A—H11A	0.88 (4)	C5A—C6A	1.389 (8)
C1—C2	1.404 (9)	C2A—H2A	0.9300
C1—C11	1.515 (9)	C3A—H3A	0.9300
C1—C6	1.397 (9)	C5A—H5A	0.9300
C2—C21	1.523 (7)	C6A—H6A	0.9300
C11—O12—H12	110 (2)	O22—C21—C2	117.9 (5)
H11A—N1A—H12A	110 (4)	O21—C21—C2	114.6 (5)
H11A—N1A—H13A	109 (4)	C2—C3—H3	120.00
C1A—N1A—H13A	108 (3)	C4—C3—H3	120.00
C1A—N1A—H11A	109 (3)	C5—C6—H6	120.00
H12A—N1A—H13A	111 (4)	C1—C6—H6	120.00
C6—C1—C11	117.1 (6)	C2A—C1A—C6A	120.9 (5)
C2—C1—C11	122.5 (5)	N1A—C1A—C6A	119.3 (4)
C2—C1—C6	120.4 (5)	N1A—C1A—C2A	119.8 (5)
C1—C2—C3	118.8 (5)	C1A—C2A—C3A	119.4 (6)
C3—C2—C21	118.2 (5)	C2A—C3A—C4A	119.1 (6)
C1—C2—C21	122.9 (5)	C14A—C4A—C3A	120.4 (5)
C2—C3—C4	120.6 (6)	C14A—C4A—C5A	117.1 (5)
C3—C4—C5	119.7 (6)	C3A—C4A—C5A	122.5 (6)
C14—C4—C5	121.7 (5)	C4A—C5A—C6A	117.6 (6)
C14—C4—C3	118.6 (5)	C1A—C6A—C5A	120.5 (5)
C15—C5—C6	118.9 (5)	C1A—C2A—H2A	120.00
C4—C5—C6	120.2 (6)	C3A—C2A—H2A	120.00
C15—C5—C4	120.9 (5)	C2A—C3A—H3A	120.00
C1—C6—C5	120.2 (6)	C4A—C3A—H3A	120.00
O11—C11—C1	121.7 (6)	C4A—C5A—H5A	121.00
O11—C11—O12	125.1 (6)	C6A—C5A—H5A	121.00
O12—C11—C1	113.1 (6)	C1A—C6A—H6A	120.00
O21—C21—O22	127.4 (5)	C5A—C6A—H6A	120.00
C6—C1—C2—C3	1.2 (10)	C2—C3—C4—C5	-0.7 (10)
C6—C1—C2—C21	-179.6 (6)	C14—C4—C5—C15	3.1 (9)
C11—C1—C2—C3	177.4 (6)	C14—C4—C5—C6	-179.6 (5)
C11—C1—C2—C21	-3.4 (10)	C3—C4—C5—C15	-176.9 (5)
C2—C1—C6—C5	-1.4 (10)	C3—C4—C5—C6	0.5 (10)
C11—C1—C6—C5	-177.8 (6)	C15—C5—C6—C1	177.9 (5)
C2—C1—C11—O11	163.7 (7)	C4—C5—C6—C1	0.5 (10)
C2—C1—C11—O12	-17.4 (9)	N1A—C1A—C2A—C3A	-177.1 (6)
C6—C1—C11—O11	-20.0 (10)	C6A—C1A—C2A—C3A	1.5 (10)
C6—C1—C11—O12	159.0 (6)	N1A—C1A—C6A—C5A	177.6 (6)
C1—C2—C3—C4	-0.2 (10)	C2A—C1A—C6A—C5A	-0.9 (10)
C21—C2—C3—C4	-179.4 (6)	C1A—C2A—C3A—C4A	-0.8 (10)
C1—C2—C21—O21	100.2 (7)	C2A—C3A—C4A—C14A	179.7 (5)
C1—C2—C21—O22	-83.3 (8)	C2A—C3A—C4A—C5A	-0.5 (10)
C3—C2—C21—O21	-80.6 (7)	C14A—C4A—C5A—C6A	-179.1 (5)
C3—C2—C21—O22	95.9 (7)	C3A—C4A—C5A—C6A	1.0 (10)
C2—C3—C4—C14	179.4 (5)	C4A—C5A—C6A—C1A	-0.3 (10)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
O12—H12···O21 ⁱ	0.81 (3)	1.69 (3)	2.485 (5)	166 (4)
N1A—H11A···O11 ⁱⁱ	0.89 (4)	2.03 (4)	2.867 (8)	157 (4)
N1A—H11A···O22	0.89 (4)	2.59 (4)	2.875 (7)	100 (2)
N1A—H12A···O22	0.88 (3)	2.58 (5)	2.875 (7)	100 (3)
N1A—H12A···O22 ⁱⁱⁱ	0.88 (3)	1.94 (3)	2.813 (6)	172 (5)
N1A—H13A···O12 ^{iv}	0.88 (4)	2.58 (5)	3.019 (7)	112 (3)
N1A—H13A···O21 ^{iv}	0.88 (4)	1.94 (4)	2.805 (7)	166 (4)
C5A—H5A···O21 ^v	0.93	2.45	3.212 (8)	139

Symmetry codes: (i) $-x+3/2, y-1/2, -z+2$; (ii) $x, y+1, z$; (iii) $-x+1, y, -z+2$; (iv) $x-1/2, y+1/2, z$; (v) $x-1/2, y-1/2, z$.