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4-Methoxyanilinium 2-carboxy-4,5-dichlorobenzoate

Graham Smith* and Urs D. Wermuth

Science and Engineering Faculty, Queensland University of Technology, GPO Box 2434, Brisbane, Queensland 4001, Australia
Correspondence e-mail: g.smith@qut.edu.au

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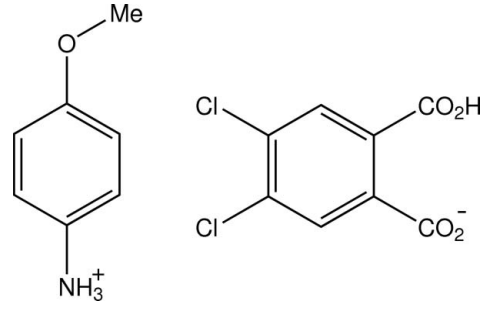
Key indicators: single-crystal X-ray study; T = 200 K; mean σ(C–C) = 0.007 Å; R factor = 0.067; wR factor = 0.117; data-to-parameter ratio = 13.1.

In the title salt $C_7H_{10}NO^+\cdot C_8H_3Cl_2O_4^-$ the benzene rings of the cation and anion are essentially parallel [inter-ring dihedral angle 4.8 (2)°]. In the anion the carboxylic acid and carboxylate groups make dihedral angles of 19.0 (2) and 79.5 (2)°, respectively, with the benzene ring. Aminium N—H···O, carboxylic acid O—H···O and weak aromatic C—H···O hydrogen-bonding associations with carboxyl O-atom acceptors together with cation–anion π–π ring interactions [minimum ring centroid separation = 3.734 (3) Å] give rise to a sheet structure lying parallel to (001).

Related literature

For background to 4,5-dichlorophthalate salts, see: Mattes & Dorau (1986); Smith *et al.* (2008*a*). For structures of some 1:1 anilinium salts of 4,5-dichlorophthalic acid, see: Odabaşoğlu & Büyükgüngör (2007); Smith *et al.* (2008*b*); Smith *et al.* (2009). For the structure of a dianionic 4,5-dichlorophthalate salt, see: Smith & Wermuth (2012).



Experimental

Crystal data

$C_7H_{10}NO^+\cdot C_8H_3Cl_2O_4^-$
M_r = 358.16
Orthorhombic, $C222_1$
a = 7.5319 (8) Å
b = 12.9302 (14) Å
c = 32.3268 (18) Å
V = 3148.3 (5) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.44 mm^{-1}
T = 200 K
0.35 × 0.30 × 0.15 mm

Data collection

Oxford Diffraction Gemini-S CCD-detector diffractometer
Absorption correction: multi-scan (*CrysAlis PRO*, Agilent, 2012)
T_{min} = 0.759, T_{max} = 0.980
6518 measured reflections
2730 independent reflections
2620 reflections with $I > 2\sigma(I)$
R_{int} = 0.036

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.067
$wR(F^2)$ = 0.117
S = 1.42
2730 reflections
208 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}
Absolute structure: Flack (1983), 1569 Friedel pairs
Absolute structure parameter: 0.03 (13)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1A—H11A···O22^{i}	0.81	2.10	2.881 (5)	163
N1A—H12A···O11^{ii}	0.87	1.95	2.811 (5)	168
N1A—H13A···O12	0.99	1.84	2.814 (5)	167
O21—H21···O12^{ii}	0.95	1.53	2.480 (4)	179
C3A—H3A···O12^{iii}	0.95	2.50	3.265 (7)	137

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

Data collection: *CrysAlis PRO* (Agilent, 2012); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008) within *ORTEP-3 for Windows* (Farrugia, 2012); 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: SJ5350).

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supporting information

Acta Cryst. (2013). E**69**, o1546 [doi:10.1107/S1600536813025014]

4-Methoxyanilinium 2-carboxy-4,5-dichlorobenzoate

Graham Smith and Urs D. Wermuth

S1. Comment

4,5-Dichlorophthalic acid (DCPA) most commonly forms 1:1 salts with organic Lewis bases, often giving low-dimensional hydrogen-bonded structures (Mattes & Dorau, 1986; Smith *et al.*, 2008*a*). The 1:2 DCPA salts are uncommon, as is the presence of water molecules of solvation, an example being the benzylamine salt (a monohydrate) (Smith & Wermuth, 2012). The salts with the aniline analogues are also not common, *e.g.* with 3-(trifluoromethyl)aniline (Odabaşoğlu & Büyükgüngör, 2007), the three isomeric carboxylanilines (Smith *et al.*, 2008*b* and 2-chloroaniline (Smith *et al.*, 2009). Our 1:1 stoichiometric reaction of DCPA with 4-methoxyaniline (*p*-anisidine) gave the anhydrous 1:1 salt $C_7H_{10}NO^+$ $C_8H_3Cl_2O_4^-$, the title compound, and the structure is reported herein.

In this structure (Fig. 1), the DCPA anion does not have the 'planar′ conformation which is found in a large number of the 1:1 structures, but has the carboxylic acid and carboxylate groups rotated out of the benzene plane forming dihedral angles of 19.0 (2)° and 79.5 (2)°, respectively, with it. These correspond to torsion angles C1—C2—C21—O21 and C2—C1—C11—O11 of 19.1 (6) and 81.2 (5)°. In the crystal the cation and anion rings are close to parallel [inter-ring dihedral angle = 4.8 (2)°], giving layering along *b*. Weak *π*–*π* interactions are present between the benzene rings of the cations and anions [minimum ring centroid separation $Cg\cdots Cg^{iv}$ = 3.734 (3) Å] [for symmetry code (iv): *x* + 1/2, *y* + 1/2, *z*]. Aminium N—H···O, water O—H···O and weak aromatic C—H···O hydrogen-bonding associations with carboxyl O-atom acceptors (Table 1) give a two-dimensional sheet structure which lies parallel to (001) (Fig. 2).

S2. Experimental

The title compound was synthesized by heating together for 10 min under reflux, 1 mmol quantities of 4,5-dichlorophthalic acid and 4-methoxyaniline (*p*-anisidine) in 50 ml of methanol. Partial evaporation of the solvent gave large colourless crystalline plates of the title compound (m.p. 473 K) from which a specimen was cleaved for the X-ray analysis..

S3. Refinement

The aminium and carboxylic acid hydrogen atoms were located by difference methods but in the final refinement cycles these were allowed to ride on the parent atom, with U_{iso}(H) = 1.2U_{eq}(N) or 1.5U_{eq}(O)]. Other H atoms were included at calculated positions [C—H (aromatic) = 0.95 Å or C—H (methyl) = 0.98 Å] and allowed to ride, with U_{iso}(H) = 1.2 or 1.5U_{eq}(C), respectively. Although not of great importance in this achiral molecule, the Flack parameter (Flack, 1983) was determined as 0.03 (13) for 1569 Friedel pairs. The TwinRotMat check [*PLATON* (Spek, 2009)] indicated no applicable twin law.

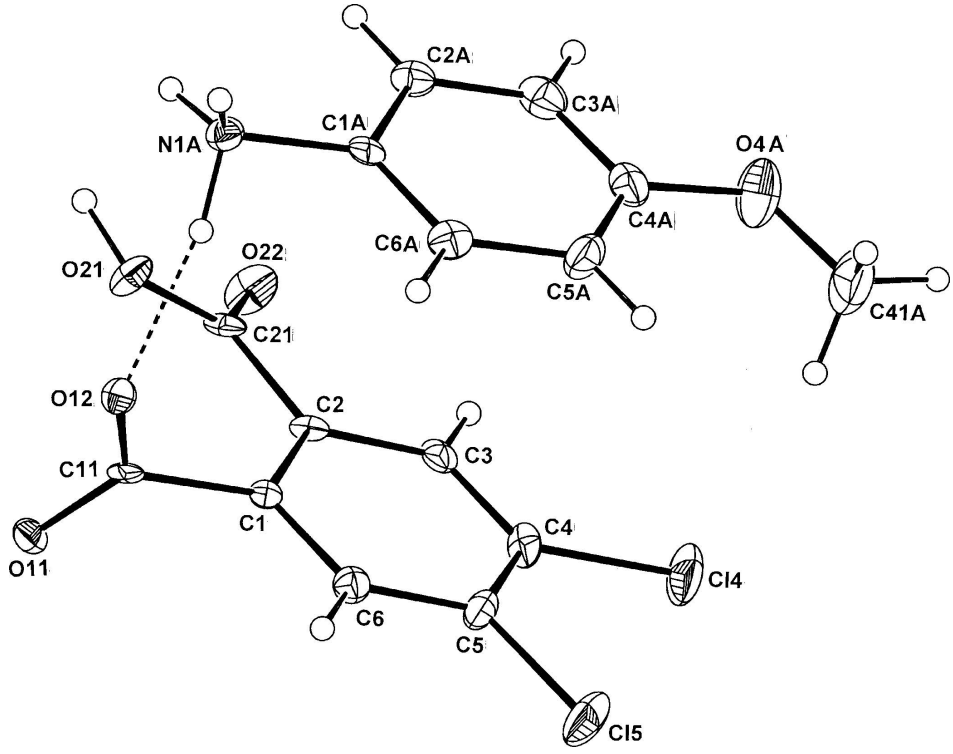

Figure 1

Molecular conformation and atom-numbering scheme for the cation and anion in the title salt, with the inter-species hydrogen bond shown as a dashed line. Non-H atoms are shown with 40% probability displacement ellipsoids.

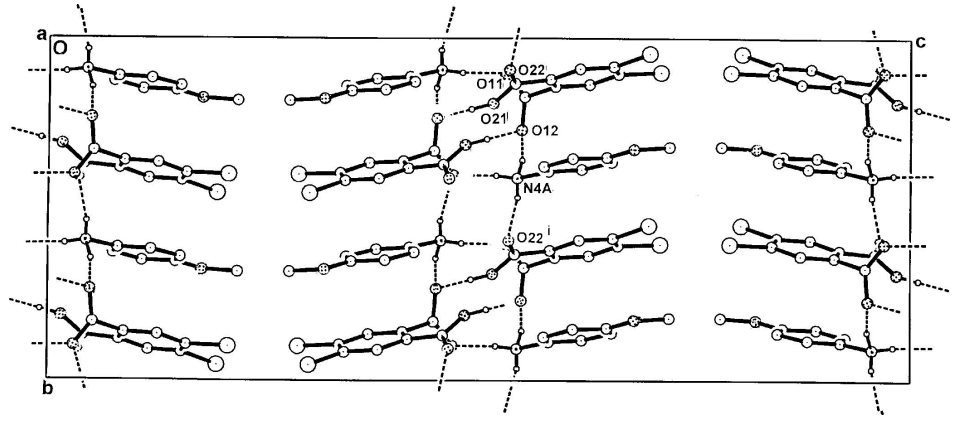

Figure 2

The two-dimensional structure in the unit cell viewed down the polymer layer, showing hydrogen-bonding associations as dashed lines. Non-associative H-atoms are omitted.

4-Methoxyanilinium 2-carboxy-4,5-dichlorobenzoate

Crystal data

$C_7H_{10}NO^+·C_8H_3Cl_2O_4^-$
M_r = 358.16
Orthorhombic, $C222_1$
Hall symbol: C 2c 2

a = 7.5319 (8) Å
b = 12.9302 (14) Å
c = 32.3268 (18) Å
V = 3148.3 (5) Å^3

$Z = 8$
$F(000) = 1472$
$D_x = 1.511$ Mg m^{-3}
Melting point: 473 K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2436 reflections

$\theta = 3.7–28.1°$
$\mu = 0.44$ mm^{-1}
$T = 200$ K
Plate, colourless
0.35 × 0.30 × 0.15 mm

Data collection

Oxford Diffraction Gemini-S CCD-detector diffractometer
Radiation source: Enhance (Mo) X-ray source
Graphite monochromator
Detector resolution: 16.077 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*CrysAlis PRO*, Agilent, 2012)
$T_{min} = 0.759$, $T_{max} = 0.980$

6518 measured reflections
2730 independent reflections
2620 reflections with $I > 2\sigma(I)$
$R_{int} = 0.036$
$\theta_{max} = 25.0°$, $\theta_{min} = 3.1°$
$h = -8 \rightarrow 8$
$k = -15 \rightarrow 16$
$l = -38 \rightarrow 38$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.067$
$wR(F^2) = 0.117$
$S = 1.42$
2730 reflections
208 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-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0003P)^2 + 10.2538P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.32$ e Å^{-3}
$\Delta\rho_{min} = -0.33$ e Å^{-3}
Absolute structure: Flack (1983), 1569 Friedel pairs
Absolute structure parameter: 0.03 (13)

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl4	1.0614 (2)	0.04524 (14)	0.69649 (4)	0.0504 (5)
Cl5	0.6536 (2)	0.09989 (13)	0.70946 (4)	0.0482 (5)
O11	0.5402 (5)	0.1011 (3)	0.53015 (10)	0.0269 (11)
O12	0.5633 (4)	0.2669 (2)	0.54919 (9)	0.0213 (10)
O21	0.9047 (5)	0.1895 (3)	0.51574 (10)	0.0281 (11)
O22	1.1354 (5)	0.0921 (3)	0.53458 (11)	0.0380 (12)
C1	0.7212 (6)	0.1407 (3)	0.58796 (14)	0.0170 (14)
C2	0.9001 (5)	0.1197 (3)	0.58236 (14)	0.0147 (12)
C3	1.0023 (7)	0.0889 (4)	0.61632 (14)	0.0240 (16)

C4	0.9274 (7)	0.0827 (4)	0.65531 (15)	0.0270 (17)
C5	0.7505 (8)	0.1047 (4)	0.66078 (13)	0.0263 (16)
C6	0.6454 (7)	0.1346 (4)	0.62745 (13)	0.0233 (16)
C11	0.6000 (6)	0.1710 (4)	0.55224 (14)	0.0163 (12)
C21	0.9909 (6)	0.1314 (3)	0.54121 (15)	0.0200 (16)
O4A	1.2905 (6)	0.3233 (4)	0.67922 (14)	0.0607 (19)
N1A	0.8469 (5)	0.4080 (3)	0.54416 (11)	0.0233 (11)
C1A	0.9599 (6)	0.3876 (3)	0.58068 (14)	0.0203 (14)
C2A	1.1396 (7)	0.3733 (4)	0.57540 (15)	0.0270 (17)
C3A	1.2440 (8)	0.3499 (4)	0.60887 (18)	0.0350 (17)
C4A	1.1695 (8)	0.3463 (4)	0.64817 (18)	0.0333 (19)
C5A	0.9921 (8)	0.3605 (5)	0.65369 (16)	0.037 (2)
C6A	0.8838 (7)	0.3818 (4)	0.61917 (15)	0.0270 (17)
C41A	1.2233 (11)	0.3165 (6)	0.71999 (19)	0.072 (3)
H3	1.12410	0.07220	0.61260	0.0290*
H6	0.52360	0.15070	0.63140	0.0280*
H21	0.96620	0.20640	0.49100	0.0420*
H2A	1.19110	0.37960	0.54870	0.0320*
H3A	1.36690	0.33630	0.60520	0.0420*
H5A	0.94160	0.35610	0.68060	0.0450*
H6A	0.75970	0.39200	0.62250	0.0330*
H11A	0.80350	0.46520	0.54470	0.0280*
H12A	0.89410	0.40030	0.51980	0.0280*
H13A	0.75460	0.35580	0.54990	0.0280*
H41A	1.32010	0.29960	0.73910	0.1080*
H42A	1.13250	0.26230	0.72130	0.1080*
H43A	1.17060	0.38290	0.72790	0.1080*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl4	0.0580 (10)	0.0630 (11)	0.0301 (7)	0.0060 (9)	−0.0209 (7)	0.0088 (7)
Cl5	0.0724 (11)	0.0539 (10)	0.0182 (6)	0.0038 (9)	0.0077 (7)	0.0036 (7)
O11	0.031 (2)	0.0218 (18)	0.0280 (17)	−0.0087 (16)	−0.0101 (16)	0.0035 (16)
O12	0.0197 (18)	0.0207 (18)	0.0236 (16)	0.0035 (15)	−0.0036 (15)	0.0038 (14)
O21	0.027 (2)	0.036 (2)	0.0213 (17)	0.0074 (17)	0.0072 (15)	0.0107 (15)
O22	0.030 (2)	0.044 (2)	0.040 (2)	0.017 (2)	0.0067 (18)	0.0123 (19)
C1	0.026 (3)	0.005 (2)	0.020 (2)	−0.0021 (19)	−0.003 (2)	0.0001 (19)
C2	0.010 (2)	0.006 (2)	0.028 (2)	0.0044 (18)	0.0030 (19)	0.0034 (18)
C3	0.028 (3)	0.014 (2)	0.030 (3)	−0.006 (2)	−0.008 (2)	0.001 (2)
C4	0.038 (3)	0.014 (3)	0.029 (3)	0.006 (2)	−0.016 (3)	0.003 (2)
C5	0.041 (3)	0.022 (3)	0.016 (2)	0.000 (3)	−0.002 (2)	0.002 (2)
C6	0.024 (3)	0.022 (3)	0.024 (2)	0.000 (2)	−0.001 (2)	0.000 (2)
C11	0.007 (2)	0.019 (2)	0.023 (2)	−0.0040 (19)	0.0051 (18)	0.005 (2)
C21	0.016 (3)	0.011 (2)	0.033 (3)	−0.003 (2)	0.002 (2)	0.006 (2)
O4A	0.061 (3)	0.075 (4)	0.046 (3)	0.013 (3)	−0.024 (2)	0.010 (2)
N1A	0.027 (2)	0.020 (2)	0.0228 (19)	−0.0015 (19)	0.0007 (18)	0.0026 (18)
C1A	0.028 (3)	0.007 (2)	0.026 (2)	−0.006 (2)	−0.003 (2)	−0.001 (2)

C2A	0.022 (3)	0.026 (3)	0.033 (3)	−0.001 (2)	0.003 (2)	0.002 (2)
C3A	0.030 (3)	0.027 (3)	0.048 (3)	−0.001 (3)	−0.004 (3)	0.000 (3)
C4A	0.039 (4)	0.019 (3)	0.042 (3)	−0.003 (3)	−0.018 (3)	0.004 (2)
C5A	0.054 (4)	0.038 (4)	0.020 (3)	−0.004 (3)	0.002 (2)	0.002 (2)
C6A	0.033 (3)	0.016 (3)	0.032 (3)	0.003 (2)	0.004 (2)	−0.002 (2)
C41A	0.108 (7)	0.065 (5)	0.043 (4)	−0.007 (5)	−0.030 (4)	0.016 (4)

Geometric parameters (Å, º)

Cl4—C4	1.739 (5)	C3—C4	1.383 (7)
Cl5—C5	1.736 (5)	C4—C5	1.374 (8)
O11—C11	1.237 (6)	C5—C6	1.392 (7)
O12—C11	1.274 (6)	C3—H3	0.9500
O21—C21	1.290 (6)	C6—H6	0.9500
O22—C21	1.220 (6)	C1A—C6A	1.372 (7)
O21—H21	0.9500	C1A—C2A	1.377 (7)
O4A—C41A	1.415 (8)	C2A—C3A	1.371 (8)
O4A—C4A	1.388 (7)	C3A—C4A	1.390 (8)
N1A—C1A	1.479 (6)	C4A—C5A	1.361 (9)
N1A—H13A	0.9900	C5A—C6A	1.409 (7)
N1A—H11A	0.8100	C2A—H2A	0.9500
N1A—H12A	0.8700	C3A—H3A	0.9500
C1—C11	1.523 (6)	C5A—H5A	0.9500
C1—C6	1.401 (6)	C6A—H6A	0.9500
C1—C2	1.386 (6)	C41A—H41A	0.9800
C2—C3	1.399 (6)	C41A—H42A	0.9800
C2—C21	1.503 (6)	C41A—H43A	0.9800
C21—O21—H21	115.00	C2—C3—H3	120.00
C4A—O4A—C41A	116.9 (5)	C4—C3—H3	120.00
H11A—N1A—H12A	107.00	C1—C6—H6	120.00
C1A—N1A—H13A	98.00	C5—C6—H6	120.00
H12A—N1A—H13A	112.00	C2A—C1A—C6A	121.1 (4)
H11A—N1A—H13A	110.00	N1A—C1A—C6A	119.6 (4)
C1A—N1A—H12A	118.00	N1A—C1A—C2A	119.4 (4)
C1A—N1A—H11A	112.00	C1A—C2A—C3A	119.7 (5)
C2—C1—C11	122.3 (4)	C2A—C3A—C4A	119.8 (5)
C6—C1—C11	117.5 (4)	O4A—C4A—C3A	113.8 (5)
C2—C1—C6	120.3 (4)	O4A—C4A—C5A	125.4 (5)
C1—C2—C21	122.5 (4)	C3A—C4A—C5A	120.8 (5)
C1—C2—C3	119.2 (4)	C4A—C5A—C6A	119.4 (5)
C3—C2—C21	118.2 (4)	C1A—C6A—C5A	119.1 (5)
C2—C3—C4	120.5 (5)	C1A—C2A—H2A	120.00
C3—C4—C5	120.1 (5)	C3A—C2A—H2A	120.00
Cl4—C4—C3	118.5 (4)	C2A—C3A—H3A	120.00
Cl4—C4—C5	121.5 (4)	C4A—C3A—H3A	120.00
Cl5—C5—C6	118.2 (4)	C4A—C5A—H5A	120.00
C4—C5—C6	120.6 (4)	C6A—C5A—H5A	120.00

Cl5—C5—C4	121.1 (4)	C1A—C6A—H6A	120.00
C1—C6—C5	119.3 (5)	C5A—C6A—H6A	120.00
O11—C11—O12	126.0 (4)	O4A—C41A—H41A	110.00
O11—C11—C1	117.9 (4)	O4A—C41A—H42A	110.00
O12—C11—C1	116.0 (4)	O4A—C41A—H43A	109.00
O21—C21—O22	125.4 (5)	H41A—C41A—H42A	109.00
O21—C21—C2	113.2 (4)	H41A—C41A—H43A	109.00
O22—C21—C2	121.3 (4)	H42A—C41A—H43A	109.00
C41A—O4A—C4A—C5A	−1.5 (9)	C2—C3—C4—Cl4	−179.4 (4)
C41A—O4A—C4A—C3A	−178.9 (5)	C2—C3—C4—C5	1.4 (8)
C6—C1—C2—C21	−176.1 (4)	Cl4—C4—C5—C6	180.0 (4)
C6—C1—C2—C3	2.2 (6)	C3—C4—C5—Cl5	−178.8 (4)
C2—C1—C6—C5	−1.6 (7)	Cl4—C4—C5—Cl5	2.0 (7)
C11—C1—C6—C5	178.4 (4)	C3—C4—C5—C6	−0.8 (8)
C2—C1—C11—O11	81.2 (6)	C4—C5—C6—C1	0.9 (8)
C2—C1—C11—O12	−101.9 (5)	Cl5—C5—C6—C1	179.0 (4)
C6—C1—C11—O11	−98.9 (5)	N1A—C1A—C2A—C3A	−177.2 (4)
C11—C1—C2—C3	−177.8 (4)	C6A—C1A—C2A—C3A	1.9 (7)
C11—C1—C2—C21	3.8 (6)	N1A—C1A—C6A—C5A	178.9 (5)
C6—C1—C11—O12	78.0 (5)	C2A—C1A—C6A—C5A	−0.2 (7)
C1—C2—C21—O21	19.1 (6)	C1A—C2A—C3A—C4A	−3.5 (8)
C1—C2—C21—O22	−163.9 (4)	C2A—C3A—C4A—O4A	−179.1 (5)
C21—C2—C3—C4	176.3 (4)	C2A—C3A—C4A—C5A	3.4 (8)
C3—C2—C21—O22	17.8 (6)	O4A—C4A—C5A—C6A	−178.9 (5)
C3—C2—C21—O21	−159.3 (4)	C3A—C4A—C5A—C6A	−1.7 (9)
C1—C2—C3—C4	−2.1 (7)	C4A—C5A—C6A—C1A	0.1 (8)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1*A*—H11*A*···O11^{i}	0.81	2.55	2.926 (5)	110
N1*A*—H11*A*···O22^{ii}	0.81	2.10	2.881 (5)	163
N1*A*—H12*A*···O11^{iii}	0.87	1.95	2.811 (5)	168
N1*A*—H13*A*···O12	0.99	1.84	2.814 (5)	167
O21—H21···O12^{iii}	0.95	1.53	2.480 (4)	179
C3*A*—H3*A*···O12^{iv}	0.95	2.50	3.265 (7)	137

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