

Cyclohexane-1,4-dicarboxylic acid–pyridinium-4-olate (1/1)

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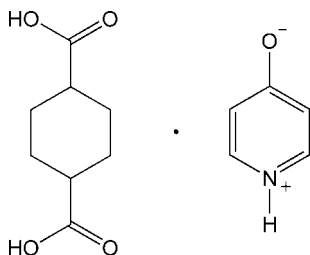
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.072; wR factor = 0.161; data-to-parameter ratio = 13.0.

In the title adduct, $\text{C}_5\text{H}_5\text{NO}\cdot\text{C}_8\text{H}_{12}\text{O}_4$, the heterocycle exists in its zwitterionic form. The cyclohexane ring exhibits a chair conformation with the carboxylic acid groups in equatorial and axial orientations. In the crystal, molecules are linked through charge-assisted $\text{O}-\text{H}\cdots\text{O}^-$, $\text{N}^+-\text{H}\cdots\text{O}^-$ and $\text{N}^+-\text{H}\cdots\text{O}$ hydrogen bonds, and an additional series of $\text{C}-\text{H}\cdots\text{O}$ contacts, giving a pleated two-dimensional hydrogen-bonded network parallel to $(\bar{2}04)$.

Related literature

For reports on supramolecular crystal engineering and potential applications of co-crystals, see: Desiraju (1995); Simon & Bassoul (2000); Weyna *et al.* (2009); Aakeröy *et al.* (2010); Yan *et al.* (2012). For related structures, see: Bhogala *et al.* (2005); Shattock *et al.* (2008); Yu (2012).



Experimental

Crystal data

$\text{C}_5\text{H}_5\text{NO}\cdot\text{C}_8\text{H}_{12}\text{O}_4$
 $M_r = 267.28$
Monoclinic, $P2_1/c$
 $a = 11.749$ (2) Å
 $b = 11.618$ (2) Å
 $c = 10.8010$ (19) Å
 $\beta = 115.383$ (2)°

$V = 1332.0$ (4) Å³
 $Z = 4$
Mo $K\alpha$ radiation
 $\mu = 0.10$ mm⁻¹
 $T = 293$ K
 $0.50 \times 0.43 \times 0.24$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
 $T_{\min} = 0.95$, $T_{\max} = 0.98$
12552 measured reflections
2345 independent reflections
2229 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.041$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.072$
 $wR(F^2) = 0.161$
 $S = 1.02$
2345 reflections
181 parameters
3 restraints

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\text{max}} = 0.20$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.27$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{O1}-\text{H1}^i\cdots\text{O5}$	0.84	1.82	2.638 (3)	165
$\text{O3}-\text{H3}^i\cdots\text{O5}^i$	0.84	1.76	2.594 (2)	175
$\text{N1}-\text{H1}\cdots\text{O4}^{ii}$	0.84	2.29	2.921 (3)	132
$\text{N1}-\text{H1}\cdots\text{O5}^{iii}$	0.84	2.39	3.038 (3)	134
$\text{C1}-\text{H1A}\cdots\text{O2}^{iv}$	0.98	2.67	3.625 (4)	162
$\text{C11}-\text{H11}\cdots\text{O2}^{iii}$	0.93	2.62	3.420 (5)	143
$\text{C12}-\text{H12}\cdots\text{O4}^{ii}$	0.93	2.47	3.014 (4)	117

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT-Plus-NT* (Bruker, 2001); data reduction: *SAINT-Plus-NT*; program(s) used to solve structure: *SHELXTL-NT* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL-NT*; molecular graphics: *ORTEP-3* (Farrugia, 2012) and *Mercury* (Macrae *et al.* 2008); software used to prepare material for publication: *pubCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PK2472).

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supporting information

Acta Cryst. (2013). E69, o591 [doi:10.1107/S160053681300754X]

Cyclohexane-1,4-dicarboxylic acid–pyridinium-4-olate (1/1)

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S1. Comment

The engineering of novel materials *via* non-covalent synthesis has developed as a very attractive and potential area of research because of its importance in biological systems, molecular recognition (Simon *et al.*, 2000; Aakeröy *et al.*, 2010), pharmaceutical chemistry (Weyna *et al.*, 2009) and materials chemistry (Yan *et al.*, 2012). Aromatic carboxylic acids form reliable supramolecular synthons for the construction of novel organic networks by hydrogen bonding and π - π interactions (Desiraju, 1995), and numerous studies have focused on hydrogen bonding between carboxylic acids and pyridine derivatives (Bhogala *et al.*, 2005; Shattock *et al.* 2008; Yu, 2012). Herein, we report on the solid-state structure of a 1:1 co-crystal formed between cyclohexane-1,4-dicarboxylic acid and pyridin-4-ol. The molecular components of the title compound are shown in Fig. 1. The asymmetric unit contains one cyclohexane-1,4-dicarboxylic acid and one pyridin-4-ol molecule in the zwitterionic form. The cyclohexane ring exhibits a chair conformation with the carboxylic groups in equatorial and axial orientation, as denoted by the C7—C1—C2—C3 [-177.7 (2)°] and C8—C4—C5—C6 [75.7 (3)°] torsion angles, respectively. In the crystal, the molecular entities are linked through charge-assisted O—H \cdots O⁻, N⁺—H \cdots O⁻ and N⁺—H \cdots O hydrogen bonds and an additional series of C—H \cdots O contacts to give a pleated two-dimensional hydrogen-bonded network parallel to (-204) (Fig. 2, Table 1).

S2. Experimental

C₅H₅NO.C₈H₁₂O₄ was prepared from a solution of C₅H₅NO (0.05 g, 0.53 mmol) and C₈H₁₂O₄ (0.09 g, 0.53 mmol) in CH₃OH (5 ml), which was stirred for a few minutes at room temperature, giving a clear transparent solution. After evaporation of the solvent, colorless crystals suitable for single-crystal X-ray diffraction had formed in about 51% yield. IR (KBr): 3471, 3276, 3131, 3092, 2937, 2863, 1709, 1632, 1576, 1509, 1416, 1364, 1331, 1316, 1229, 1170, 1001 cm⁻¹.

S3. Refinement

H atoms were found in difference Fourier maps. Carbon-bound hydrogen atoms were placed in idealized positions using a riding models with constrained distances of 0.97 Å (R₂CH₂), 0.98 Å (R₃CH) and 0.93 Å (C_{sp2}H). Coordinates for hydrogens bound to oxygen and nitrogen were refined. U_{iso}(H) values were set to either 1.2U_{eq} or 1.5U_{eq} (OH, NH) of the attached atom.

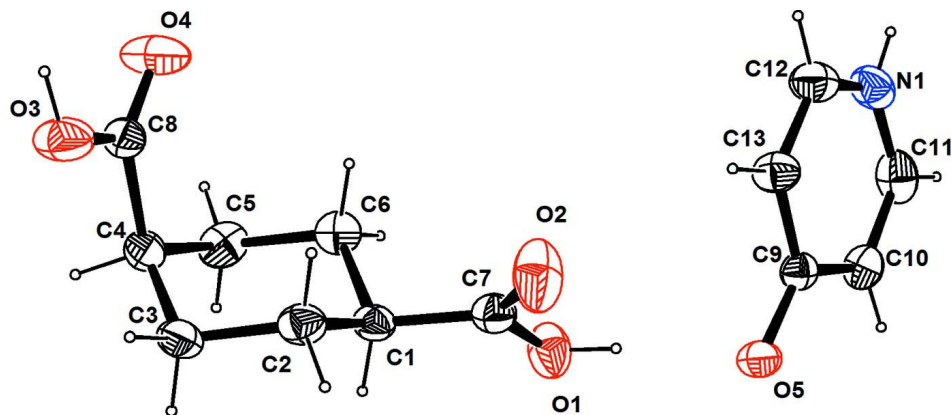


Figure 1

The molecular structures of the components in the title compound, showing displacement ellipsoids drawn at the 30% probability level.

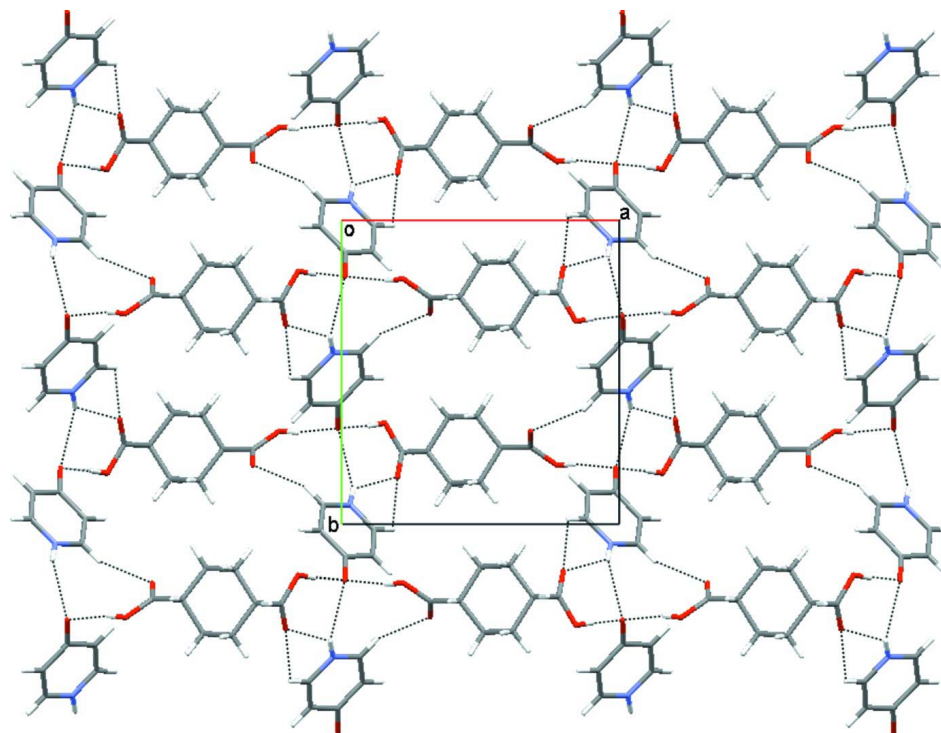


Figure 2

View down the *c*-axis of the two-dimensional hydrogen-bonded supramolecular network formed through O—H \cdots O, N⁺—H \cdots O and N⁺—H \cdots O and C—H \cdots O interactions.

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Crystal data

$C_5H_5NO \cdot C_8H_{12}O_4$

$M_r = 267.28$

Monoclinic, $P2_1/c$

Hall symbol: $-P 2_1/c$

$a = 11.749 (2) \text{ \AA}$

$b = 11.618 (2) \text{ \AA}$

$c = 10.8010 (19) \text{ \AA}$

$\beta = 115.383 (2)^\circ$

$V = 1332.0 (4) \text{ \AA}^3$

$Z = 4$

$F(000) = 568$
 $D_x = 1.333 \text{ Mg m}^{-3}$
 Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
 Cell parameters from 5484 reflections
 $\theta = 2.6\text{--}27.4^\circ$

$\mu = 0.10 \text{ mm}^{-1}$
 $T = 293 \text{ K}$
 Rectangular prism, yellow
 $0.50 \times 0.43 \times 0.24 \text{ mm}$

Data collection

Bruker SMART CCD area-detector
 diffractometer
 Radiation source: fine-focus sealed tube
 Graphite monochromator
 φ and ω scans
 Absorption correction: multi-scan
 (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.95, T_{\max} = 0.98$

12552 measured reflections
 2345 independent reflections
 2229 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.041$
 $\theta_{\max} = 25.0^\circ, \theta_{\min} = 1.9^\circ$
 $h = -13 \rightarrow 13$
 $k = -13 \rightarrow 13$
 $l = -12 \rightarrow 12$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.072$
 $wR(F^2) = 0.161$
 $S = 1.02$
 2345 reflections
 181 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
 $w = 1/[\sigma^2(F_o^2) + (0.0623P)^2 + 1.4075P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.20 \text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.27 \text{ e \AA}^{-3}$

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>	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.2230 (2)	0.1930 (2)	0.0632 (2)	0.0663 (6)
H1'	0.162 (2)	0.198 (4)	0.085 (4)	0.099*
O2	0.3186 (2)	0.3059 (3)	0.2412 (3)	0.0898 (9)
O3	0.8439 (2)	0.3327 (2)	0.3413 (2)	0.0733 (7)
H3'	0.901 (3)	0.324 (4)	0.4210 (17)	0.110*
O4	0.7984 (2)	0.15562 (19)	0.3701 (2)	0.0805 (8)
C1	0.4258 (2)	0.2522 (2)	0.1037 (2)	0.0420 (6)
H1A	0.3892	0.2539	0.0033	0.050*
C2	0.5129 (3)	0.3552 (2)	0.1563 (3)	0.0489 (7)
H2A	0.4647	0.4256	0.1246	0.059*
H2B	0.5510	0.3555	0.2557	0.059*

C3	0.6155 (3)	0.3511 (3)	0.1063 (3)	0.0556 (8)
H3A	0.6718	0.4160	0.1442	0.067*
H3B	0.5773	0.3583	0.0073	0.067*
C4	0.6915 (3)	0.2400 (3)	0.1470 (3)	0.0497 (7)
H4	0.7428	0.2374	0.0955	0.060*
C5	0.6058 (3)	0.1347 (3)	0.1039 (3)	0.0557 (8)
H5A	0.5683	0.1283	0.0048	0.067*
H5B	0.6559	0.0662	0.1416	0.067*
C6	0.5018 (3)	0.1405 (2)	0.1514 (3)	0.0485 (7)
H6A	0.5384	0.1363	0.2506	0.058*
H6B	0.4460	0.0751	0.1152	0.058*
C7	0.3195 (3)	0.2542 (2)	0.1453 (3)	0.0471 (6)
C8	0.7822 (2)	0.2371 (2)	0.2978 (3)	0.0442 (6)
N1	0.0308 (3)	-0.0636 (2)	0.3628 (3)	0.0590 (7)
H1	0.041 (4)	-0.115 (2)	0.421 (3)	0.088*
O5	0.01175 (16)	0.18473 (15)	0.09311 (18)	0.0470 (5)
C9	0.0146 (2)	0.1065 (2)	0.1791 (2)	0.0384 (6)
C10	-0.0764 (3)	0.0194 (2)	0.1462 (3)	0.0495 (7)
H10	-0.1444	0.0185	0.0603	0.059*
C11	-0.0659 (3)	-0.0638 (2)	0.2390 (4)	0.0609 (8)
H11	-0.1266	-0.1213	0.2159	0.073*
C12	0.1179 (3)	0.0179 (3)	0.4004 (3)	0.0584 (8)
H12	0.1836	0.0165	0.4880	0.070*
C13	0.1124 (3)	0.1029 (2)	0.3127 (3)	0.0497 (7)
H13	0.1740	0.1599	0.3410	0.060*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0561 (13)	0.0868 (16)	0.0593 (13)	-0.0227 (12)	0.0280 (11)	-0.0188 (12)
O2	0.0729 (16)	0.130 (2)	0.0779 (16)	-0.0249 (15)	0.0433 (14)	-0.0510 (16)
O3	0.0722 (15)	0.0658 (14)	0.0532 (13)	-0.0221 (12)	-0.0005 (11)	0.0129 (11)
O4	0.1024 (19)	0.0580 (14)	0.0471 (12)	-0.0139 (13)	-0.0003 (12)	0.0119 (11)
C1	0.0442 (14)	0.0476 (15)	0.0296 (12)	-0.0022 (11)	0.0115 (11)	0.0003 (11)
C2	0.0532 (16)	0.0370 (14)	0.0506 (15)	0.0012 (12)	0.0166 (13)	0.0067 (12)
C3	0.0529 (16)	0.0624 (18)	0.0448 (15)	-0.0094 (14)	0.0146 (13)	0.0164 (13)
C4	0.0479 (15)	0.0695 (19)	0.0349 (13)	0.0017 (14)	0.0207 (12)	0.0011 (13)
C5	0.0569 (17)	0.0591 (18)	0.0447 (15)	0.0045 (14)	0.0157 (13)	-0.0176 (13)
C6	0.0550 (16)	0.0374 (14)	0.0483 (15)	-0.0063 (12)	0.0175 (13)	-0.0069 (12)
C7	0.0480 (15)	0.0490 (16)	0.0400 (14)	-0.0005 (12)	0.0146 (12)	0.0019 (12)
C8	0.0437 (14)	0.0500 (16)	0.0386 (13)	0.0008 (12)	0.0174 (11)	0.0004 (12)
N1	0.0757 (18)	0.0480 (15)	0.0647 (17)	0.0093 (13)	0.0411 (15)	0.0138 (12)
O5	0.0441 (10)	0.0454 (10)	0.0432 (10)	-0.0014 (8)	0.0109 (8)	0.0082 (8)
C9	0.0411 (13)	0.0345 (13)	0.0403 (13)	0.0048 (10)	0.0182 (11)	-0.0015 (10)
C10	0.0450 (15)	0.0467 (16)	0.0554 (16)	-0.0027 (12)	0.0202 (13)	-0.0062 (13)
C11	0.0667 (19)	0.0407 (16)	0.088 (2)	-0.0111 (14)	0.0458 (19)	-0.0066 (15)
C12	0.0672 (19)	0.0558 (18)	0.0488 (16)	0.0103 (16)	0.0217 (14)	0.0081 (14)
C13	0.0517 (15)	0.0439 (15)	0.0449 (14)	-0.0043 (12)	0.0125 (12)	-0.0001 (12)

Geometric parameters (Å, °)

O1—C7	1.310 (3)	C4—H4	0.9800
O1—H1'	0.8400 (10)	C5—C6	1.516 (4)
O2—C7	1.201 (3)	C5—H5A	0.9700
O3—C8	1.299 (3)	C5—H5B	0.9700
O3—H3'	0.8400 (11)	C6—H6A	0.9700
O4—C8	1.189 (3)	C6—H6B	0.9700
C1—C7	1.498 (4)	N1—C12	1.324 (4)
C1—C2	1.518 (4)	N1—C11	1.333 (4)
C1—C6	1.534 (4)	N1—H1	0.8400 (10)
C1—H1A	0.9800	O5—C9	1.289 (3)
C2—C3	1.518 (4)	C9—C10	1.403 (4)
C2—H2A	0.9700	C9—C13	1.408 (4)
C2—H2B	0.9700	C10—C11	1.359 (4)
C3—C4	1.524 (4)	C10—H10	0.9300
C3—H3A	0.9700	C11—H11	0.9300
C3—H3B	0.9700	C12—C13	1.351 (4)
C4—C8	1.517 (4)	C12—H12	0.9300
C4—C5	1.525 (4)	C13—H13	0.9300
C7—O1—H1'	112 (3)	H5A—C5—H5B	107.8
C8—O3—H3'	110 (3)	C5—C6—C1	111.2 (2)
C7—C1—C2	113.0 (2)	C5—C6—H6A	109.4
C7—C1—C6	110.6 (2)	C1—C6—H6A	109.4
C2—C1—C6	109.8 (2)	C5—C6—H6B	109.4
C7—C1—H1A	107.7	C1—C6—H6B	109.4
C2—C1—H1A	107.7	H6A—C6—H6B	108.0
C6—C1—H1A	107.7	O2—C7—O1	122.0 (3)
C3—C2—C1	110.7 (2)	O2—C7—C1	125.7 (3)
C3—C2—H2A	109.5	O1—C7—C1	112.3 (2)
C1—C2—H2A	109.5	O4—C8—O3	122.4 (2)
C3—C2—H2B	109.5	O4—C8—C4	124.3 (3)
C1—C2—H2B	109.5	O3—C8—C4	113.3 (2)
H2A—C2—H2B	108.1	C12—N1—C11	121.6 (3)
C2—C3—C4	112.4 (2)	C12—N1—H1	116 (3)
C2—C3—H3A	109.1	C11—N1—H1	122 (3)
C4—C3—H3A	109.1	O5—C9—C10	123.0 (2)
C2—C3—H3B	109.1	O5—C9—C13	121.1 (2)
C4—C3—H3B	109.1	C10—C9—C13	115.8 (2)
H3A—C3—H3B	107.9	C11—C10—C9	120.6 (3)
C8—C4—C3	112.5 (2)	C11—C10—H10	119.7
C8—C4—C5	112.2 (2)	C9—C10—H10	119.7
C3—C4—C5	111.2 (2)	N1—C11—C10	120.5 (3)
C8—C4—H4	106.8	N1—C11—H11	119.8
C3—C4—H4	106.8	C10—C11—H11	119.8
C5—C4—H4	106.8	N1—C12—C13	120.6 (3)
C6—C5—C4	112.6 (2)	N1—C12—H12	119.7

C6—C5—H5A	109.1	C13—C12—H12	119.7
C4—C5—H5A	109.1	C12—C13—C9	120.9 (3)
C6—C5—H5B	109.1	C12—C13—H13	119.6
C4—C5—H5B	109.1	C9—C13—H13	119.6
C7—C1—C2—C3	-177.7 (2)	C6—C1—C7—O1	-79.7 (3)
C6—C1—C2—C3	58.2 (3)	C3—C4—C8—O4	136.9 (3)
C1—C2—C3—C4	-56.6 (3)	C5—C4—C8—O4	10.5 (4)
C2—C3—C4—C8	-74.5 (3)	C3—C4—C8—O3	-44.6 (3)
C2—C3—C4—C5	52.4 (3)	C5—C4—C8—O3	-170.9 (2)
C8—C4—C5—C6	75.7 (3)	O5—C9—C10—C11	177.2 (2)
C3—C4—C5—C6	-51.4 (3)	C13—C9—C10—C11	-1.8 (4)
C4—C5—C6—C1	54.4 (3)	C12—N1—C11—C10	1.2 (4)
C7—C1—C6—C5	177.2 (2)	C9—C10—C11—N1	0.3 (4)
C2—C1—C6—C5	-57.4 (3)	C11—N1—C12—C13	-1.1 (5)
C2—C1—C7—O2	-22.5 (4)	N1—C12—C13—C9	-0.5 (4)
C6—C1—C7—O2	101.1 (3)	O5—C9—C13—C12	-177.1 (3)
C2—C1—C7—O1	156.7 (2)	C10—C9—C13—C12	1.9 (4)

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>
O1—H1'...O5	0.84	1.82	2.638 (3)	165
O3—H3'...O5 ⁱ	0.84	1.76	2.594 (2)	175
N1—H1...O4 ⁱⁱ	0.84	2.29	2.921 (3)	132
N1—H1...O5 ⁱⁱⁱ	0.84	2.39	3.038 (3)	134
C1—H1A...O2 ^{iv}	0.98	2.67	3.625 (4)	162
C11—H11...O2 ⁱⁱⁱ	0.93	2.62	3.420 (5)	143
C12—H12...O4 ⁱⁱ	0.93	2.47	3.014 (4)	117

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