Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

catena-Poly[[bis[(2-carboxybenzoato-κO)silver(I)](*Ag*—*Ag*)]bis(*μ*-isonicotinic acid-$\kappa^2 N$:*O*)]

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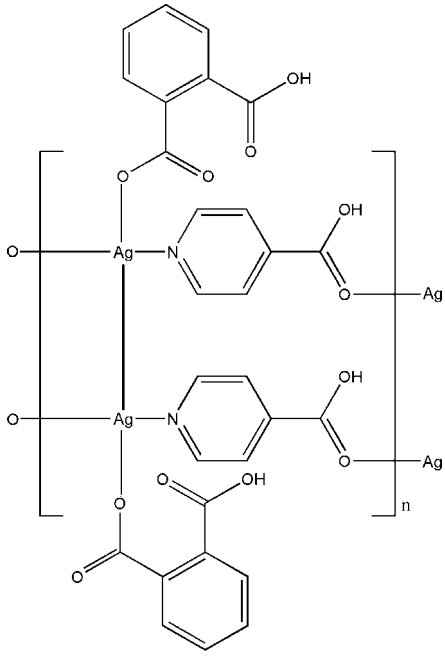
Received 20 February 2008; accepted 7 April 2008

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.006 Å; R factor = 0.043; wR factor = 0.120; data-to-parameter ratio = 15.3.

The title compound, $[Ag(C_8H_5O_4)(C_6H_5NO_2)]_n$, contains one Ag^I atom, one phthalate ligand and one isonicotinic acid molecule in the asymmetric unit. Each Ag atom is three-coordinated in a T-shaped geometry by two O atoms and one N atom from one phthalate ligand and two isonicotinic acid ligands. The isonicotinic acid ligand bridges two Ag atoms, forming a one-dimensional chain. Adjacent chains are linked by Ag—Ag interactions, leading to a double-chain. These double-chains are further linked *via* hydrogen bonds into a two-dimensional layer.

Related literature

For related literature, see: He *et al.* (2007); Xie *et al.* (2005).



Experimental

Crystal data

$[Ag(C_8H_5O_4)(C_6H_5NO_2)]$
M_r = 396.10
Monoclinic, $C2/c$
a = 13.540 (3) Å
b = 8.160 (2) Å
c = 24.223 (5) Å
β = 99.546 (15)°
V = 2639 (1) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 1.56 mm^{-1}
T = 293 (2) K
0.37 × 0.32 × 0.27 mm

Data collection

Siemens P4 four-circle diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.597, T_{max} = 0.680
3909 measured reflections
3037 independent reflections
1879 reflections with $I > 2\sigma(I)$
R_{int} = 0.034
3 standard reflections
every 97 reflections
intensity decay: 1.0%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.119
S = 1.00
3037 reflections
199 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.99 e Å^{-3}
$\Delta\rho_{min}$ = −0.71 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ag1—N1	2.179 (4)	Ag1—O2^{i}	2.621 (3)
Ag1—O3	2.185 (3)	Ag1—Ag1^{ii}	3.2123 (11)
N1—Ag1—O3	164.57 (14)	O3—Ag1—O2^{i}	101.74 (11)
N1—Ag1—O2^{i}	93.52 (12)		

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

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1A···O6^{iii}	0.82	1.80	2.616 (5)	175
O5—H5A···O4	0.82	1.57	2.390 (5)	180

Symmetry code: (iii) $x, -y+1, z-\frac{1}{2}$.

Data collection: *XSCANS* (Siemens, 1994); cell refinement: *XSCANS*; data reduction: *XSCANS*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2008).

The authors thank Shanghai Maritime University for supporting this work.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2121).

References

Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
He, Y.-K., Han, Z.-B., Ma, Y. & Zhang, X.-D. (2007). *Inorg. Chem. Commun.* **10**, 829–832.
North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* A**24**, 351–359.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Siemens (1994). *XSCANS*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Westrip, S. P. (2008). *publCIF*. In preparation.
Xie, F.-T., Bie, H.-Y., Duan, L.-M., Li, G.-H., Zhang, X. & Xu, J.-Q. (2005). *J. Solid State Chem.* **178**, 2858–2866.

supporting information

Acta Cryst. (2008). E**64**, m779 [doi:10.1107/S1600536808009586]

catena-Poly[[bis[(2-carboxybenzoato-κO)silver(I)](*Ag*—*Ag*)]bis(μ-isonicotinic acid-$\kappa^2 N$:*O*)]

Xiao-Feng Li, Yan An and Yan-Sheng Yin

S1. Comment

Silver ion reacts with isonicotinic acid and imidazole under hydrothermal conditions to form $[Ag_8(in)_6(NO_3)_2]$ and $[Ag(in)(Hin)]_{0.5}[Ag(in)]$ (Hin = isonicotinic acid) (Xie *et al.*, 2005). With phthalic acid in place of imidazole, the reaction yields the title compound.

In the title compound, the Ag^I atom is three-coordinated by two O atoms and one N atom from one phthalate ligand and two isonicotinic acid ligands in a T-like geometry, with an O—Ag—N bond angle being 164.57 (14)° (Fig. 1; Table 1), giving a chain structure. Furthermore, the adjacent chains are linked by Ag···Ag interactions (He *et al.*, 2007) to form a one-dimensional double-chain (Fig. 2). These double-chains are further linked *via* O—H···O hydrogen bonds (Table 2) into a two-dimensional layer. The hydrogen bonding interactions enhance the stability of the complex.

S2. Experimental

A mixture of $Ag(NO_3)$ (0.085 g, 0.5 mmol), isonicotinic acid (0.123 g, 1 mmol), phthalic acid (0.166 g, 1 mmol) and water (10 ml) was sealed in a 23 ml Teflon-lined reactor, which was heated at 473 K for 4 d and then cooled to room temperature at a rate of 5 K h^{-1} (yield 72%). Analysis calculated for $C_{14}H_{10}AgNO_6$: C 42.45, H 2.54, N 3.54%; found: C 42.39, H 2.61, N 3.48%.

S3. Refinement

H atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93 and O—H = 0.82Å and U_{iso}(H) = 1.2U_{eq}(C,*O*).

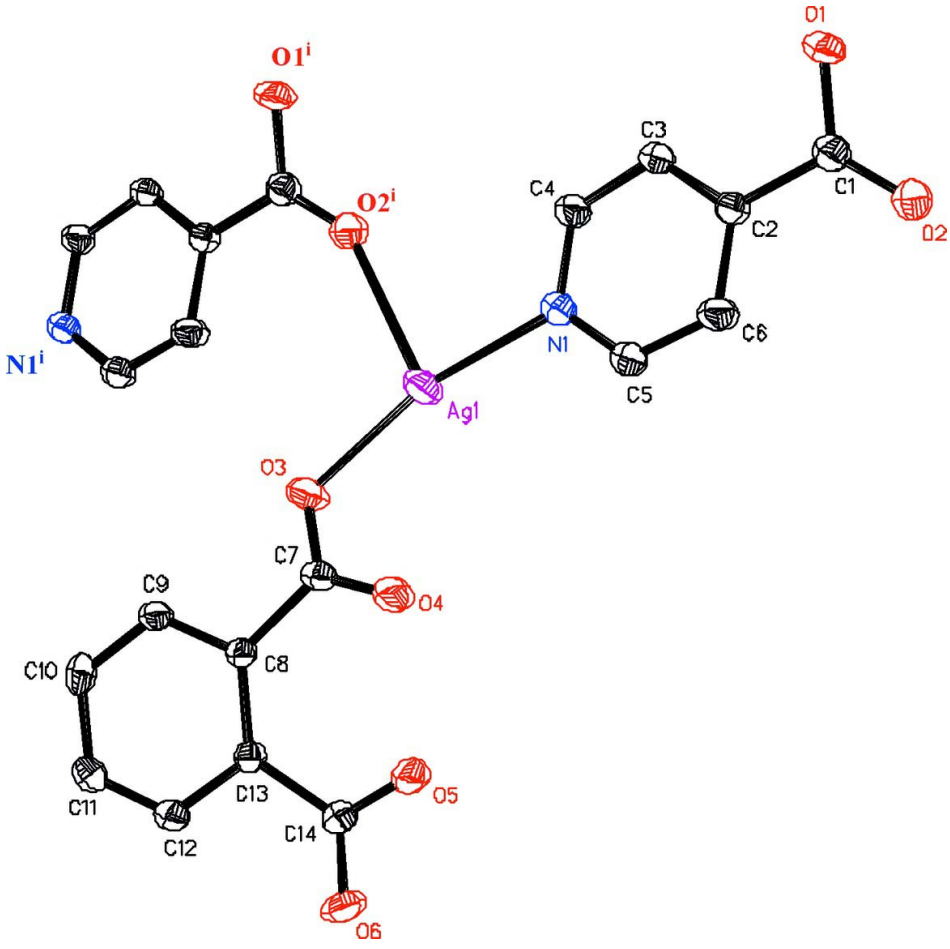


Figure 1

The coordination geometry of the Ag atom in the title compound. Displacement ellipsoids are drawn at the 30% probability level. [Symmetry code: (i) *x*, -1 + *y*, *z*.]

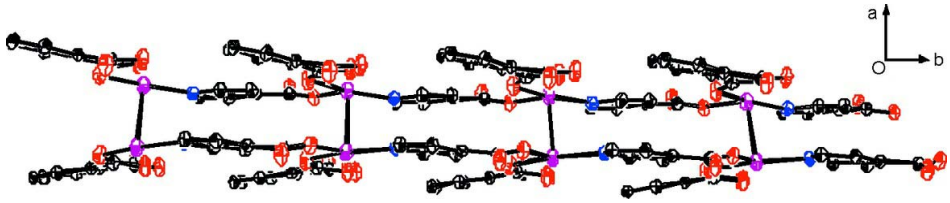


Figure 2

The one-dimensional double-chain connected by Ag···Ag interactions.

catena-Poly[[bis[(2-carboxybenzoato-κO)silver(I)](Ag—Ag)]bis(μ-isonicotinic acid-$\kappa^2 N$:O)]

Crystal data

$[Ag(C_8H_5O_4)(C_6H_5NO_2)]$
M_r = 396.10
Monoclinic, *C*2/*c*
Hall symbol: -C 2yc
a = 13.540 (3) Å
b = 8.160 (2) Å
c = 24.223 (5) Å
β = 99.546 (15)°
V = 2639 (1) Å^3
Z = 8
F(000) = 1568
D_x = 1.994 Mg m^{-3}

Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 28 reflections
θ = 5.2–12.4°
μ = 1.56 mm^{-1}
T = 293 K
Block, purple
0.37 × 0.32 × 0.27 mm

Data collection

Siemens P4 four-circle diffractometer
Radiation source: medium-focus sealed tube
Graphite monochromator
ω–2θ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.597, T_{max} = 0.680
3909 measured reflections
3037 independent reflections
1879 reflections with $I > 2\sigma(I)$
R_{int} = 0.034
θ_{max} = 27.5°, θ_{min} = 1.7°
h = −17→1
k = −1→10
l = −31→31
3 standard reflections every 97 reflections
intensity decay: 1.0%

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.119
S = 1.00
3037 reflections
199 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
$w = 1/[\sigma^2(F_o^2) + (0.0526P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.99 e Å^{-3}
$\Delta\rho_{min}$ = −0.72 e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Ag1	0.40822 (3)	0.04719 (5)	0.698630 (15)	0.05417 (17)
C1	0.4164 (4)	0.7535 (6)	0.58243 (19)	0.0405 (11)
C2	0.4211 (3)	0.5872 (5)	0.60835 (17)	0.0347 (10)
C3	0.4339 (4)	0.4453 (6)	0.57882 (17)	0.0397 (10)
H3A	0.4417	0.4514	0.5415	0.048*
C4	0.4348 (4)	0.2962 (6)	0.60478 (18)	0.0413 (11)
H4A	0.4430	0.2020	0.5844	0.050*
C5	0.4137 (4)	0.4183 (6)	0.68640 (19)	0.0442 (12)
H5B	0.4070	0.4087	0.7239	0.053*
C6	0.4119 (4)	0.5724 (6)	0.66396 (19)	0.0455 (12)
H6A	0.4046	0.6644	0.6856	0.055*
C7	0.3575 (4)	−0.0952 (6)	0.80056 (17)	0.0383 (11)
C8	0.3373 (3)	−0.2215 (5)	0.84252 (16)	0.0307 (9)
C9	0.3225 (3)	−0.3796 (6)	0.82196 (17)	0.0368 (10)
H9A	0.3240	−0.3975	0.7842	0.044*
C10	0.3056 (4)	−0.5119 (6)	0.8547 (2)	0.0437 (11)
H10A	0.2958	−0.6164	0.8394	0.052*
C11	0.3036 (4)	−0.4842 (6)	0.9109 (2)	0.0453 (12)
H11A	0.2927	−0.5711	0.9340	0.054*
C12	0.3177 (4)	−0.3304 (6)	0.93258 (18)	0.0403 (11)
H12A	0.3159	−0.3145	0.9704	0.048*

C13	0.3346 (3)	−0.1963 (5)	0.89994 (17)	0.0321 (9)
C14	0.3497 (4)	−0.0355 (6)	0.93203 (18)	0.0411 (11)
N1	0.4245 (3)	0.2820 (5)	0.65827 (15)	0.0414 (9)
O1	0.3992 (3)	0.7496 (5)	0.52779 (12)	0.0626 (11)
H1A	0.3896	0.8431	0.5156	0.094*
O2	0.4267 (3)	0.8778 (4)	0.60899 (13)	0.0513 (9)
O3	0.3817 (3)	−0.1459 (4)	0.75691 (13)	0.0579 (10)
O4	0.3483 (3)	0.0565 (4)	0.80925 (14)	0.0619 (11)
O5	0.3438 (3)	0.1015 (4)	0.90631 (14)	0.0579 (10)
H5A	0.3454	0.0858	0.8730	0.087*
O6	0.3672 (3)	−0.0408 (4)	0.98320 (13)	0.0641 (11)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ag1	0.0797 (3)	0.0432 (2)	0.0430 (2)	0.0001 (2)	0.02032 (19)	0.01176 (18)
C1	0.046 (3)	0.038 (3)	0.037 (2)	0.002 (2)	0.007 (2)	0.002 (2)
C2	0.037 (2)	0.037 (2)	0.030 (2)	−0.001 (2)	0.0055 (18)	0.0028 (18)
C3	0.055 (3)	0.036 (2)	0.028 (2)	−0.003 (2)	0.008 (2)	0.0023 (19)
C4	0.055 (3)	0.037 (2)	0.034 (2)	0.000 (2)	0.012 (2)	−0.0002 (19)
C5	0.061 (3)	0.039 (3)	0.034 (2)	−0.002 (2)	0.012 (2)	0.0022 (19)
C6	0.065 (3)	0.042 (3)	0.031 (2)	0.005 (3)	0.014 (2)	−0.002 (2)
C7	0.046 (3)	0.042 (3)	0.027 (2)	−0.001 (2)	0.0060 (19)	0.0026 (19)
C8	0.038 (2)	0.028 (2)	0.0250 (18)	−0.0007 (19)	0.0035 (17)	0.0007 (17)
C9	0.050 (3)	0.034 (2)	0.0278 (19)	−0.001 (2)	0.0098 (19)	−0.0021 (18)
C10	0.045 (3)	0.027 (2)	0.057 (3)	−0.003 (2)	0.004 (2)	−0.001 (2)
C11	0.058 (3)	0.037 (3)	0.042 (2)	−0.005 (2)	0.009 (2)	0.010 (2)
C12	0.051 (3)	0.040 (3)	0.030 (2)	−0.003 (2)	0.007 (2)	0.0033 (19)
C13	0.038 (2)	0.028 (2)	0.031 (2)	0.002 (2)	0.0056 (18)	0.0000 (17)
C14	0.053 (3)	0.036 (3)	0.035 (2)	−0.004 (2)	0.012 (2)	−0.006 (2)
N1	0.053 (2)	0.038 (2)	0.0349 (18)	−0.0020 (19)	0.0101 (18)	0.0034 (17)
O1	0.112 (3)	0.042 (2)	0.0295 (16)	−0.002 (2)	−0.0001 (19)	0.0104 (15)
O2	0.075 (3)	0.0364 (18)	0.0425 (18)	0.0043 (19)	0.0082 (17)	0.0005 (16)
O3	0.101 (3)	0.0417 (19)	0.0379 (17)	0.004 (2)	0.0313 (19)	0.0044 (16)
O4	0.116 (3)	0.0339 (18)	0.0379 (17)	−0.003 (2)	0.019 (2)	0.0053 (15)
O5	0.107 (3)	0.0303 (17)	0.0380 (17)	−0.006 (2)	0.017 (2)	−0.0037 (15)
O6	0.117 (3)	0.047 (2)	0.0278 (15)	−0.004 (2)	0.0086 (19)	−0.0078 (16)

Geometric parameters (Å, º)

Ag1—N1	2.179 (4)	C7—O4	1.265 (6)
Ag1—O3	2.185 (3)	C7—C8	1.504 (6)
Ag1—O2^{i}	2.621 (3)	C8—C9	1.385 (6)
Ag1—Ag1^{ii}	3.2123 (11)	C8—C13	1.412 (5)
C1—O2	1.197 (6)	C9—C10	1.380 (6)
C1—O1	1.306 (5)	C9—H9A	0.9300
C1—C2	1.492 (6)	C10—C11	1.387 (7)
C2—C6	1.379 (6)	C10—H10A	0.9300

C2—C3	1.386 (6)	C11—C12	1.361 (7)
C3—C4	1.368 (6)	C11—H11A	0.9300
C3—H3A	0.9300	C12—C13	1.391 (6)
C4—N1	1.331 (5)	C12—H12A	0.9300
C4—H4A	0.9300	C13—C14	1.521 (6)
C5—N1	1.325 (6)	C14—O6	1.223 (5)
C5—C6	1.368 (7)	C14—O5	1.276 (6)
C5—H5B	0.9300	O1—H1A	0.8200
C6—H6A	0.9300	O5—H5A	0.8200
C7—O3	1.229 (5)		

N1—Ag1—O3	164.57 (14)	C9—C8—C7	115.3 (3)
N1—Ag1—O2^{i}	93.52 (12)	C13—C8—C7	127.1 (4)
O3—Ag1—O2^{i}	101.74 (11)	C10—C9—C8	123.4 (4)
N1—Ag1—Ag1^{ii}	102.98 (11)	C10—C9—H9A	118.3
O3—Ag1—Ag1^{ii}	71.85 (11)	C8—C9—H9A	118.3
O2—C1—O1	123.4 (4)	C9—C10—C11	117.9 (4)
O2—C1—C2	123.5 (4)	C9—C10—H10A	121.0
O1—C1—C2	113.1 (4)	C11—C10—H10A	121.0
C6—C2—C3	118.0 (4)	C12—C11—C10	120.3 (4)
C6—C2—C1	119.1 (4)	C12—C11—H11A	119.8
C3—C2—C1	122.9 (4)	C10—C11—H11A	119.8
C4—C3—C2	119.8 (4)	C11—C12—C13	122.2 (4)
C4—C3—H3A	120.1	C11—C12—H12A	118.9
C2—C3—H3A	120.1	C13—C12—H12A	118.9
N1—C4—C3	122.0 (4)	C12—C13—C8	118.6 (4)
N1—C4—H4A	119.0	C12—C13—C14	114.1 (4)
C3—C4—H4A	119.0	C8—C13—C14	127.3 (4)
N1—C5—C6	124.3 (4)	O6—C14—O5	120.8 (4)
N1—C5—H5B	117.9	O6—C14—C13	118.3 (4)
C6—C5—H5B	117.9	O5—C14—C13	120.9 (4)
C5—C6—C2	118.0 (5)	C5—N1—C4	117.8 (4)
C5—C6—H6A	121.0	C5—N1—Ag1	118.6 (3)
C2—C6—H6A	121.0	C4—N1—Ag1	123.3 (3)
O3—C7—O4	121.4 (4)	C1—O1—H1A	109.5
O3—C7—C8	117.0 (4)	C7—O3—Ag1	114.1 (3)
O4—C7—C8	121.6 (4)	C14—O5—H5A	109.5
C9—C8—C13	117.6 (4)		

O2—C1—C2—C6	16.8 (8)	C9—C8—C13—C12	0.2 (7)
O1—C1—C2—C6	−162.7 (4)	C7—C8—C13—C12	−178.0 (4)
O2—C1—C2—C3	−163.7 (5)	C9—C8—C13—C14	179.3 (4)
O1—C1—C2—C3	16.8 (7)	C7—C8—C13—C14	1.1 (8)
C6—C2—C3—C4	1.3 (7)	C12—C13—C14—O6	15.3 (7)
C1—C2—C3—C4	−178.2 (5)	C8—C13—C14—O6	−163.8 (5)
C2—C3—C4—N1	−0.5 (8)	C12—C13—C14—O5	−164.4 (5)
N1—C5—C6—C2	0.4 (8)	C8—C13—C14—O5	16.5 (8)
C3—C2—C6—C5	−1.3 (7)	C6—C5—N1—C4	0.4 (8)

C1—C2—C6—C5	178.3 (5)	C6—C5—N1—Ag1	−173.0 (4)
O3—C7—C8—C9	−16.1 (6)	C3—C4—N1—C5	−0.4 (7)
O4—C7—C8—C9	162.6 (5)	C3—C4—N1—Ag1	172.6 (4)
O3—C7—C8—C13	162.1 (5)	O3—Ag1—N1—C5	4.1 (8)
O4—C7—C8—C13	−19.2 (8)	Ag1^{ii}—Ag1—N1—C5	−64.4 (4)
C13—C8—C9—C10	−0.1 (7)	O3—Ag1—N1—C4	−168.9 (5)
C7—C8—C9—C10	178.3 (4)	Ag1^{ii}—Ag1—N1—C4	122.6 (4)
C8—C9—C10—C11	−0.1 (8)	O4—C7—O3—Ag1	0.9 (6)
C9—C10—C11—C12	0.3 (8)	C8—C7—O3—Ag1	179.6 (3)
C10—C11—C12—C13	−0.2 (8)	N1—Ag1—O3—C7	0.2 (8)
C11—C12—C13—C8	−0.1 (7)	Ag1^{ii}—Ag1—O3—C7	72.7 (4)
C11—C12—C13—C14	−179.3 (5)		

Symmetry codes: (i) *x*, *y*−1, *z*; (ii) −*x*+1, *y*, −*z*+3/2.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*A*···O6^{iii}	0.82	1.80	2.616 (5)	175
O5—H5*A*···O4	0.82	1.57	2.390 (5)	180

Symmetry code: (iii) *x*, −*y*+1, *z*−1/2.