

Crystal structure of 1,7,8,9-tetrachloro-4-(3,5-dichlorobenzyl)-10,10-dimethoxy-4-azatricyclo[5.2.1.0^{2,6}]dec-8-ene-3,5-dione

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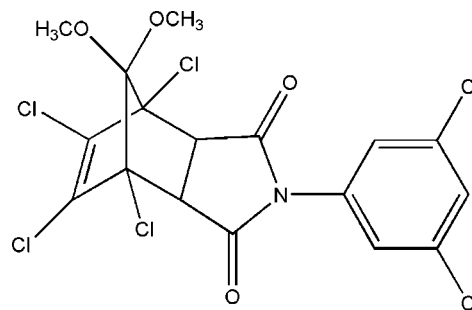
In the title compound, C₁₇H₁₁Cl₆NO₄, the configuration of the cycloalkene skeleton is *endo,cis*. The benzene ring is twisted by 58.94 (8)° from the attached pyrrolidine ring. Two carbonyl groups play a key role in the crystal packing. A short intermolecular C⋯O distance of 3.017 (3) Å reveals that one carbonyl group is involved in dipole–dipole interactions, which link two adjacent enantiomers into an inversion dimer. Another carbonyl group provides an acceptor for the weak intermolecular C–H⋯O hydrogen bonds which link these dimers into layers parallel to (011).

Keywords: crystal structure; tricyclo[5.2.1.0^{2,6}]dec-8-ene-3,5-dione; biological activity; cycloalkene skeleton; dipole–dipole interactions; hydrogen bonding.

CCDC reference: 1036270

1. Related literature

For related crystal structures, see: Shan *et al.* (2012); Kossakowski *et al.* (2009). For the biological activity of related compounds, see: Kossakowski *et al.* (2006, 2008); Struga *et al.* (2007).



2. Experimental

2.1. Crystal data

C ₁₇ H ₁₁ Cl ₆ NO ₄	$\gamma = 90.23 (3)^\circ$
$M_r = 505.97$	$V = 1015.2 (4) \text{ \AA}^3$
Triclinic, $P\bar{1}$	$Z = 2$
$a = 8.9905 (18) \text{ \AA}$	Mo $K\alpha$ radiation
$b = 11.351 (2) \text{ \AA}$	$\mu = 0.87 \text{ mm}^{-1}$
$c = 11.482 (2) \text{ \AA}$	$T = 296 \text{ K}$
$\alpha = 119.52 (3)^\circ$	$0.25 \times 0.20 \times 0.15 \text{ mm}$
$\beta = 94.51 (3)^\circ$	

2.2. Data collection

Bruker APEXII CCD diffractometer	4611 independent reflections
10037 measured reflections	3865 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.036$

2.3. Refinement

$R[F^2 > 2\sigma(F^2)] = 0.043$	254 parameters
$wR(F^2) = 0.111$	H-atom parameters constrained
$S = 1.05$	$\Delta\rho_{\text{max}} = 0.70 \text{ e \AA}^{-3}$
4611 reflections	$\Delta\rho_{\text{min}} = -0.64 \text{ e \AA}^{-3}$

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C14–H14A⋯O2 ⁱ	0.93	2.57	3.265 (4)	132
C18–H18A⋯O2 ⁱⁱ	0.96	2.45	3.260 (4)	141

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

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

Acknowledgements

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Supporting information for this paper is available from the IUCr electronic archives (Reference: CV5477).

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supporting information

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Crystal structure of 1,7,8,9-tetrachloro-4-(3,5-dichlorobenzyl)-10,10-dimethoxy-4-azatricyclo[5.2.1.0^{2,6}]dec-8-ene-3,5-dione

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S1. Comment

The title compound, (I) (Fig. 1), was synthesized from *N*-(3',5'-dichlorobenzyl)maleimide and 5,5-dimethoxy-1,2,3,4-tetrachlorocyclopentadiene. The fused pyrrolidine ring systems are frequently encountered structural units in many synthetically challenging and biologically active alkaloids. The interest of constructing skeletons of this type was further enlightened by the recent disclosure that the rigid arylcyclo analogues having azatricyclo ring systems show anti-HIV-1, anti-cancer, antiviral, and antibacterial activities (Kossakowski *et al.*, 2006).

In (I), the configuration of the cycloalkene skeleton is *endo, cis*. The dihedral angle of pyrrolidine ring and benzene ring is 58.94 (8)°. Two carbonyl groups play a key role in the crystal packing (Fig. 2). One carbonyl group is involved in dipole-dipole interactions, with C3...O1(-*x*+2, -*y*+2, -*z*) distance of 3.017 (3) Å, which link two adjacent enantiomers into inversion dimers. The other carbonyl group provides an acceptor for two weak intermolecular C—H...O hydrogen bonds (Table 1). These intermolecular interactions link these dimers into layers parallel to (011).

S2. Experimental

N-(3,5-Dichlorobenzyl)maleimide (2.44 g, 10 mmol) and 5,5-dimethoxy-1,2,3,4-tetrachlorocyclopentadiene (2.63 g, 10 mmol) were dissolved in anhydrous toluene (100 ml). Then, the solution was refluxed for 8 h. After the solvent was removed under reduced pressure, the residue was dissolved in ether (150 ml), washed with water and brine, dried over anhydrous sodium sulfate, and concentrated to dryness. The product was purified by flash-chromatography (petroleum ether/ethyl acetate, 6:1) and the title compound was isolated as a white solid (4.16 g, 82%), with melting point between 104 and 106°C.

The crystals appropriate for X-ray data collection were obtained from acetone solution at room temperature after four days.

S3. Refinement

All H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms with C—H distances of 0.93 Å (0.98 for alicyclic CH) for aromatic ring CH, and $U_{\text{iso}}(\text{H}) = 1.2\text{--}1.5 U_{\text{eq}}(\text{C})$.

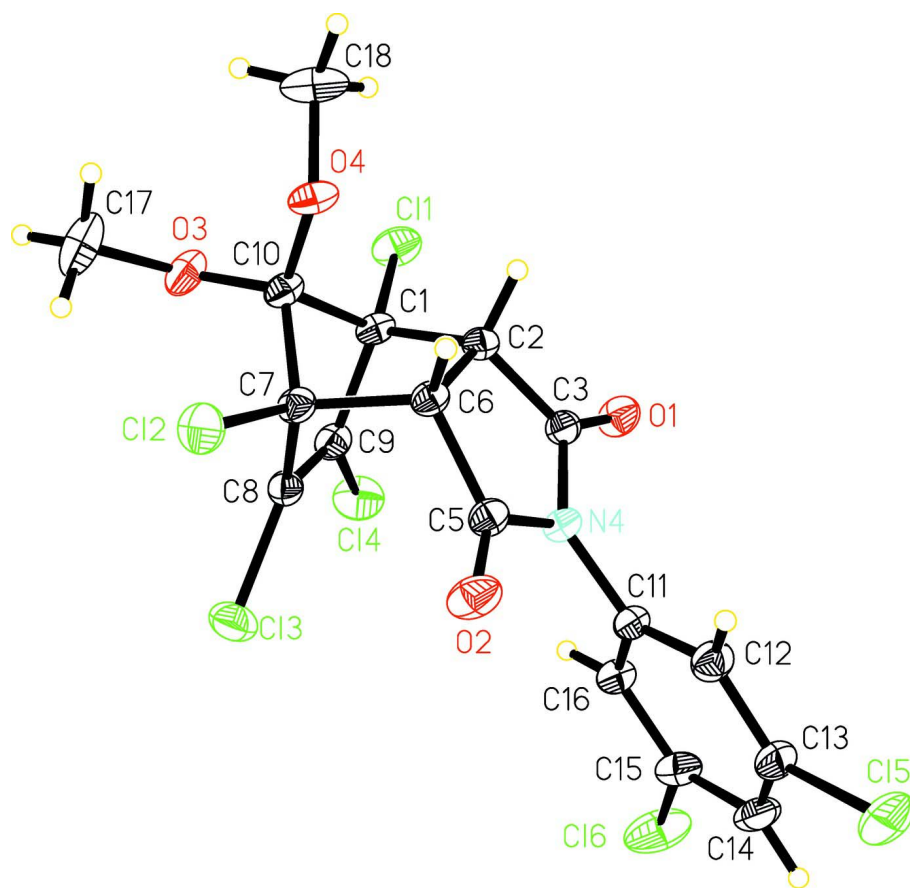


Figure 1

View of (I) showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

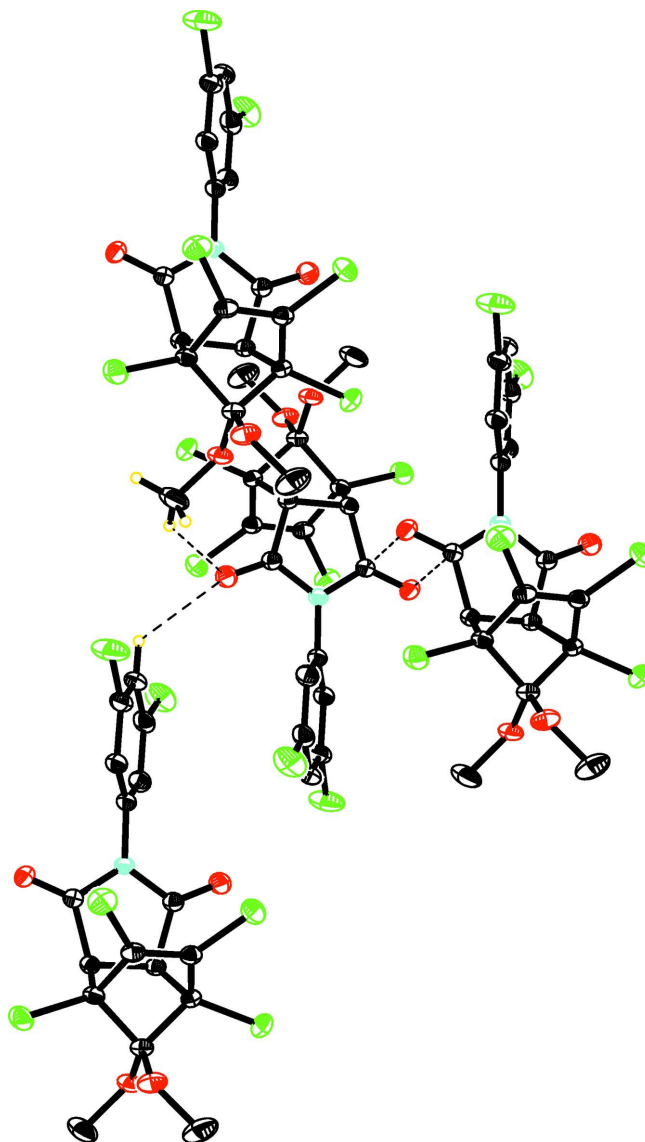


Figure 2

A portion of the crystal packing viewed approximately along [01-1]. The dipole-dipole and intermolecular C—H···O interactions are shown by dashed lines. H atoms not involved in C—H···O interactions are omitted for clarity.

1,7,8,9-Tetrachloro-4-(3,5-dichlorobenzyl)-10,10-dimethoxy-4-azatricyclo[5.2.1.0^{2,6}]dec-8-ene-3,5-dione

Crystal data

$C_{17}H_{11}Cl_6NO_4$

$M_r = 505.97$

Triclinic, $P\bar{1}$

Hall symbol: -P 1

$a = 8.9905 (18) \text{ \AA}$

$b = 11.351 (2) \text{ \AA}$

$c = 11.482 (2) \text{ \AA}$

$\alpha = 119.52 (3)^\circ$

$\beta = 94.51 (3)^\circ$

$\gamma = 90.23 (3)^\circ$

$V = 1015.2 (4) \text{ \AA}^3$

$Z = 2$

$F(000) = 508$

$D_x = 1.655 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 4035 reflections

$\theta = 3.0\text{--}27.3^\circ$

$\mu = 0.87 \text{ mm}^{-1}$

$T = 296$ K $0.25 \times 0.20 \times 0.15$ mm
 Column, colourless

Data collection

Bruker APEXII CCD diffractometer	3865 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	$R_{\text{int}} = 0.036$
Graphite monochromator	$\theta_{\text{max}} = 27.5^\circ$, $\theta_{\text{min}} = 3.0^\circ$
φ and ω scans	$h = -10 \rightarrow 11$
10037 measured reflections	$k = -14 \rightarrow 14$
4611 independent reflections	$l = -14 \rightarrow 14$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.043$	$w = 1/[\sigma^2(F_o^2) + (0.0412P)^2 + 0.6429P]$
$wR(F^2) = 0.111$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.05$	$(\Delta/\sigma)_{\text{max}} = 0.001$
4611 reflections	$\Delta\rho_{\text{max}} = 0.70 \text{ e } \text{\AA}^{-3}$
254 parameters	$\Delta\rho_{\text{min}} = -0.64 \text{ e } \text{\AA}^{-3}$
0 restraints	Extinction correction: <i>SHELXL97</i> (Sheldrick, 2008), $F_c^* = kFc[1 + 0.001x\text{Fc}^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.041 (3)
Secondary atom site location: difference Fourier map	

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)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Cl1	0.86211 (7)	0.64648 (6)	0.01529 (7)	0.04952 (18)
Cl2	0.42071 (6)	1.01968 (7)	0.22921 (7)	0.04994 (18)
Cl3	0.68066 (8)	1.06565 (7)	0.47167 (6)	0.05378 (19)
Cl4	0.95541 (7)	0.84784 (7)	0.33571 (7)	0.05465 (19)
Cl5	1.13965 (11)	1.59013 (7)	0.35138 (9)	0.0729 (3)
Cl6	1.36383 (11)	1.31140 (9)	0.58471 (9)	0.0808 (3)
O1	1.08016 (17)	0.94674 (16)	0.09979 (18)	0.0439 (4)
O2	0.72222 (19)	1.24926 (16)	0.29413 (19)	0.0498 (4)
O3	0.54476 (19)	0.70159 (18)	0.11801 (19)	0.0484 (4)
O4	0.53317 (18)	0.77943 (16)	-0.03513 (15)	0.0412 (4)
N4	0.92584 (19)	1.11941 (17)	0.21831 (17)	0.0314 (4)
C1	0.7734 (2)	0.8000 (2)	0.1025 (2)	0.0314 (4)
C2	0.8098 (2)	0.9081 (2)	0.0613 (2)	0.0298 (4)

H2A	0.8017	0.8681	-0.0367	0.036*
C3	0.9573 (2)	0.9867 (2)	0.1245 (2)	0.0314 (4)
C5	0.7731 (2)	1.1424 (2)	0.2225 (2)	0.0330 (4)
C6	0.6890 (2)	1.0109 (2)	0.1241 (2)	0.0299 (4)
H6A	0.6270	1.0203	0.0553	0.036*
C7	0.5955 (2)	0.9495 (2)	0.1918 (2)	0.0323 (4)
C8	0.6949 (2)	0.9539 (2)	0.3068 (2)	0.0335 (4)
C9	0.8003 (2)	0.8677 (2)	0.2542 (2)	0.0343 (5)
C10	0.5982 (2)	0.7951 (2)	0.0854 (2)	0.0340 (5)
C11	1.0373 (2)	1.2261 (2)	0.2981 (2)	0.0333 (4)
C12	1.0362 (3)	1.3406 (2)	0.2843 (2)	0.0409 (5)
H12A	0.9684	1.3467	0.2222	0.049*
C13	1.1394 (3)	1.4455 (2)	0.3660 (3)	0.0449 (6)
C14	1.2412 (3)	1.4386 (2)	0.4583 (3)	0.0472 (6)
H14A	1.3094	1.5104	0.5128	0.057*
C15	1.2391 (3)	1.3220 (2)	0.4674 (2)	0.0438 (5)
C16	1.1374 (2)	1.2143 (2)	0.3883 (2)	0.0371 (5)
H16A	1.1369	1.1365	0.3960	0.044*
C17	0.3854 (3)	0.6908 (4)	0.1208 (4)	0.0770 (10)
H17A	0.3617	0.6226	0.1436	0.115*
H17B	0.3366	0.6663	0.0339	0.115*
H17C	0.3516	0.7763	0.1866	0.115*
C18	0.5309 (4)	0.6462 (3)	-0.1513 (3)	0.0659 (9)
H18A	0.4837	0.6481	-0.2282	0.099*
H18B	0.4761	0.5833	-0.1356	0.099*
H18C	0.6314	0.6183	-0.1673	0.099*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C11	0.0530 (4)	0.0289 (3)	0.0557 (4)	0.0074 (2)	-0.0005 (3)	0.0132 (3)
C12	0.0286 (3)	0.0601 (4)	0.0557 (4)	0.0069 (2)	0.0054 (3)	0.0243 (3)
C13	0.0559 (4)	0.0620 (4)	0.0311 (3)	0.0005 (3)	0.0030 (3)	0.0138 (3)
C14	0.0498 (4)	0.0656 (4)	0.0509 (4)	0.0087 (3)	-0.0132 (3)	0.0330 (3)
C15	0.1059 (7)	0.0302 (3)	0.0815 (5)	-0.0056 (3)	0.0087 (5)	0.0269 (3)
C16	0.0848 (6)	0.0607 (5)	0.0737 (5)	-0.0117 (4)	-0.0449 (4)	0.0228 (4)
O1	0.0299 (8)	0.0397 (9)	0.0530 (10)	0.0028 (6)	0.0050 (7)	0.0157 (8)
O2	0.0422 (9)	0.0303 (8)	0.0605 (11)	0.0061 (7)	0.0023 (8)	0.0103 (8)
O3	0.0439 (9)	0.0454 (10)	0.0604 (11)	-0.0151 (7)	-0.0078 (8)	0.0314 (9)
O4	0.0420 (9)	0.0352 (8)	0.0356 (8)	-0.0046 (6)	-0.0142 (7)	0.0117 (7)
N4	0.0293 (9)	0.0271 (8)	0.0332 (9)	-0.0022 (6)	-0.0018 (7)	0.0121 (7)
C1	0.0332 (10)	0.0242 (9)	0.0327 (10)	-0.0013 (7)	-0.0050 (8)	0.0120 (8)
C2	0.0312 (10)	0.0291 (10)	0.0269 (9)	0.0003 (8)	-0.0012 (8)	0.0127 (8)
C3	0.0327 (11)	0.0302 (10)	0.0304 (10)	-0.0008 (8)	0.0009 (8)	0.0147 (8)
C5	0.0340 (11)	0.0291 (10)	0.0357 (10)	0.0007 (8)	-0.0008 (9)	0.0163 (9)
C6	0.0289 (10)	0.0287 (10)	0.0308 (10)	-0.0007 (7)	-0.0033 (8)	0.0147 (8)
C7	0.0259 (10)	0.0343 (11)	0.0328 (10)	-0.0009 (8)	-0.0019 (8)	0.0143 (9)
C8	0.0329 (11)	0.0382 (11)	0.0295 (10)	-0.0052 (8)	-0.0013 (8)	0.0175 (9)

C9	0.0345 (11)	0.0368 (11)	0.0354 (11)	-0.0046 (8)	-0.0063 (9)	0.0222 (9)
C10	0.0326 (11)	0.0315 (10)	0.0352 (10)	-0.0053 (8)	-0.0068 (9)	0.0159 (9)
C11	0.0337 (11)	0.0279 (10)	0.0329 (10)	-0.0038 (8)	0.0024 (8)	0.0109 (8)
C12	0.0456 (13)	0.0327 (11)	0.0433 (12)	0.0004 (9)	0.0026 (10)	0.0183 (10)
C13	0.0556 (15)	0.0258 (10)	0.0477 (13)	-0.0016 (9)	0.0114 (12)	0.0128 (10)
C14	0.0459 (14)	0.0309 (11)	0.0450 (13)	-0.0068 (9)	0.0004 (11)	0.0041 (10)
C15	0.0429 (13)	0.0364 (12)	0.0381 (11)	-0.0010 (9)	-0.0052 (10)	0.0089 (10)
C16	0.0394 (12)	0.0309 (11)	0.0360 (11)	-0.0017 (8)	-0.0003 (9)	0.0134 (9)
C17	0.0500 (17)	0.078 (2)	0.113 (3)	-0.0235 (16)	0.0000 (18)	0.056 (2)
C18	0.076 (2)	0.0465 (16)	0.0449 (15)	0.0048 (14)	-0.0211 (14)	0.0028 (13)

Geometric parameters (Å, °)

C11—C1	1.758 (2)	C5—C6	1.507 (3)
C12—C7	1.752 (2)	C6—C7	1.558 (3)
C13—C8	1.698 (2)	C6—H6A	0.9800
C14—C9	1.696 (2)	C7—C8	1.514 (3)
C15—C13	1.730 (2)	C7—C10	1.568 (3)
C16—C15	1.735 (3)	C8—C9	1.318 (3)
O1—C3	1.197 (3)	C11—C16	1.375 (3)
O2—C5	1.199 (3)	C11—C12	1.385 (3)
O3—C10	1.383 (3)	C12—C13	1.383 (3)
O3—C17	1.442 (3)	C12—H12A	0.9300
O4—C10	1.385 (3)	C13—C14	1.377 (4)
O4—C18	1.440 (3)	C14—C15	1.379 (4)
N4—C5	1.399 (3)	C14—H14A	0.9300
N4—C3	1.400 (3)	C15—C16	1.386 (3)
N4—C11	1.436 (3)	C16—H16A	0.9300
C1—C9	1.515 (3)	C17—H17A	0.9600
C1—C2	1.558 (3)	C17—H17B	0.9600
C1—C10	1.569 (3)	C17—H17C	0.9600
C2—C3	1.511 (3)	C18—H18A	0.9600
C2—C6	1.538 (3)	C18—H18B	0.9600
C2—H2A	0.9800	C18—H18C	0.9600
C10—O3—C17	117.0 (2)	C8—C9—C14	127.64 (18)
C10—O4—C18	117.17 (19)	C1—C9—C14	123.58 (17)
C5—N4—C3	113.59 (17)	O3—C10—O4	113.93 (18)
C5—N4—C11	121.92 (17)	O3—C10—C7	118.24 (19)
C3—N4—C11	124.39 (18)	O4—C10—C7	106.81 (17)
C9—C1—C2	107.61 (16)	O3—C10—C1	108.32 (17)
C9—C1—C10	100.14 (17)	O4—C10—C1	116.35 (18)
C2—C1—C10	100.16 (16)	C7—C10—C1	91.53 (15)
C9—C1—C11	114.51 (15)	C16—C11—C12	122.2 (2)
C2—C1—C11	114.82 (15)	C16—C11—N4	119.76 (19)
C10—C1—C11	117.67 (14)	C12—C11—N4	118.0 (2)
C3—C2—C6	105.59 (16)	C13—C12—C11	117.7 (2)
C3—C2—C1	114.53 (17)	C13—C12—H12A	121.2

C6—C2—C1	102.43 (16)	C11—C12—H12A	121.2
C3—C2—H2A	111.3	C14—C13—C12	122.2 (2)
C6—C2—H2A	111.3	C14—C13—C15	119.21 (19)
C1—C2—H2A	111.3	C12—C13—C15	118.6 (2)
O1—C3—N4	124.78 (19)	C13—C14—C15	118.0 (2)
O1—C3—C2	127.70 (19)	C13—C14—H14A	121.0
N4—C3—C2	107.52 (17)	C15—C14—H14A	121.0
O2—C5—N4	124.4 (2)	C14—C15—C16	122.0 (2)
O2—C5—C6	127.7 (2)	C14—C15—C16	119.06 (19)
N4—C5—C6	107.93 (17)	C16—C15—C16	118.9 (2)
C5—C6—C2	105.31 (16)	C11—C16—C15	117.9 (2)
C5—C6—C7	113.74 (17)	C11—C16—H16A	121.0
C2—C6—C7	103.90 (16)	C15—C16—H16A	121.0
C5—C6—H6A	111.2	O3—C17—H17A	109.5
C2—C6—H6A	111.2	O3—C17—H17B	109.5
C7—C6—H6A	111.2	H17A—C17—H17B	109.5
C8—C7—C6	107.50 (16)	O3—C17—H17C	109.5
C8—C7—C10	100.17 (17)	H17A—C17—H17C	109.5
C6—C7—C10	99.80 (16)	H17B—C17—H17C	109.5
C8—C7—C12	116.77 (15)	O4—C18—H18A	109.5
C6—C7—C12	112.98 (15)	O4—C18—H18B	109.5
C10—C7—C12	117.57 (15)	H18A—C18—H18B	109.5
C9—C8—C7	107.49 (18)	O4—C18—H18C	109.5
C9—C8—C13	127.66 (18)	H18A—C18—H18C	109.5
C7—C8—C13	124.45 (16)	H18B—C18—H18C	109.5
C8—C9—C1	108.25 (19)		
C9—C1—C2—C3	48.4 (2)	C11—C1—C9—C8	-160.38 (16)
C10—C1—C2—C3	152.57 (17)	C2—C1—C9—C14	-101.47 (19)
C11—C1—C2—C3	-80.38 (19)	C10—C1—C9—C14	154.36 (16)
C9—C1—C2—C6	-65.4 (2)	C11—C1—C9—C14	27.5 (2)
C10—C1—C2—C6	38.79 (18)	C17—O3—C10—O4	-54.4 (3)
C11—C1—C2—C6	165.84 (13)	C17—O3—C10—C7	72.3 (3)
C5—N4—C3—O1	176.3 (2)	C17—O3—C10—C1	174.4 (2)
C11—N4—C3—O1	-0.1 (3)	C18—O4—C10—O3	-51.2 (3)
C5—N4—C3—C2	-2.6 (2)	C18—O4—C10—C7	176.3 (2)
C11—N4—C3—C2	-178.97 (18)	C18—O4—C10—C1	75.9 (3)
C6—C2—C3—O1	-176.5 (2)	C8—C7—C10—O3	60.5 (2)
C1—C2—C3—O1	71.6 (3)	C6—C7—C10—O3	170.41 (18)
C6—C2—C3—N4	2.3 (2)	C12—C7—C10—O3	-67.1 (2)
C1—C2—C3—N4	-109.57 (19)	C8—C7—C10—O4	-169.50 (16)
C3—N4—C5—O2	-178.8 (2)	C6—C7—C10—O4	-59.55 (19)
C11—N4—C5—O2	-2.4 (3)	C12—C7—C10—O4	62.9 (2)
C3—N4—C5—C6	1.8 (2)	C8—C7—C10—C1	-51.33 (17)
C11—N4—C5—C6	178.21 (18)	C6—C7—C10—C1	58.61 (17)
O2—C5—C6—C2	-179.5 (2)	C12—C7—C10—C1	-178.91 (15)
N4—C5—C6—C2	-0.1 (2)	C9—C1—C10—O3	-70.1 (2)
O2—C5—C6—C7	-66.4 (3)	C2—C1—C10—O3	179.76 (16)

N4—C5—C6—C7	112.96 (19)	C11—C1—C10—O3	54.6 (2)
C3—C2—C6—C5	-1.3 (2)	C9—C1—C10—O4	160.04 (18)
C1—C2—C6—C5	118.88 (17)	C2—C1—C10—O4	49.9 (2)
C3—C2—C6—C7	-121.17 (17)	C11—C1—C10—O4	-75.2 (2)
C1—C2—C6—C7	-0.97 (19)	C9—C1—C10—C7	50.40 (18)
C5—C6—C7—C8	-47.1 (2)	C2—C1—C10—C7	-59.74 (17)
C2—C6—C7—C8	66.9 (2)	C11—C1—C10—C7	175.13 (15)
C5—C6—C7—C10	-151.10 (17)	C5—N4—C11—C16	121.4 (2)
C2—C6—C7—C10	-37.14 (18)	C3—N4—C11—C16	-62.5 (3)
C5—C6—C7—C12	83.22 (19)	C5—N4—C11—C12	-56.3 (3)
C2—C6—C7—C12	-162.83 (13)	C3—N4—C11—C12	119.8 (2)
C6—C7—C8—C9	-68.0 (2)	C16—C11—C12—C13	-0.6 (3)
C10—C7—C8—C9	35.8 (2)	N4—C11—C12—C13	177.0 (2)
C12—C7—C8—C9	163.88 (16)	C11—C12—C13—C14	0.2 (4)
C6—C7—C8—C13	105.23 (19)	C11—C12—C13—C15	-179.64 (17)
C10—C7—C8—C13	-151.01 (16)	C12—C13—C14—C15	0.4 (4)
C12—C7—C8—C13	-22.9 (2)	C15—C13—C14—C15	-179.70 (19)
C7—C8—C9—C1	-1.3 (2)	C13—C14—C15—C16	-0.8 (4)
C13—C8—C9—C1	-174.27 (16)	C13—C14—C15—C16	-178.90 (19)
C7—C8—C9—C14	170.36 (16)	C12—C11—C16—C15	0.3 (3)
C13—C8—C9—C14	-2.6 (3)	N4—C11—C16—C15	-177.3 (2)
C2—C1—C9—C8	70.7 (2)	C14—C15—C16—C11	0.4 (4)
C10—C1—C9—C8	-33.5 (2)	C16—C15—C16—C11	178.55 (17)

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>
C14—H14 <i>A</i> ...O2 ⁱ	0.93	2.57	3.265 (4)	132
C18—H18 <i>A</i> ...O2 ⁱⁱ	0.96	2.45	3.260 (4)	141

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