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4,5,6,7-Tetrachloro-3-(cyclohepta-1,3,6-trien-1-yl)-3-hydroxy-2-(2-hydroxyethyl)-2,3-dihydro-1*H*-isoindol-1-one

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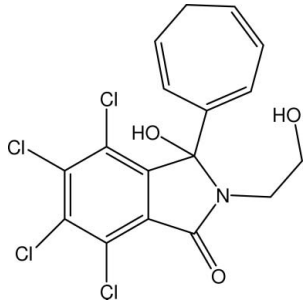
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.003 Å; disorder in main residue; R factor = 0.047; wR factor = 0.130; data-to-parameter ratio = 18.3.

In the title compound, $C_{17}H_{13}Cl_4NO_3$, the isoindole unit is essentially planar. The seven-membered ring adopts a boat conformation. The O atom of the hydroxyethyl group is disordered over two positions with essentially equal occupancies. In the crystal structure, the molecules are linked by O—H···O and O—H···Cl hydrogen bonds into a two-dimensional network parallel to the (010) plane.

Related literature

For hydrogen-bond motifs, see: Bernstein *et al.* (1995). For bond-length data, see: Allen *et al.* (1987). For related literature, see: Evans & Holmes (1991); Griesbeck *et al.* (1996); Illuminati & Mandolini (1981); Xue *et al.* (2000); Fun *et al.* (2007).



Experimental

Crystal data

$C_{17}H_{13}Cl_4NO_3$
M_r = 421.08
Monoclinic, $P2_1/c$
a = 5.7285 (3) Å
b = 27.9820 (12) Å
c = 10.7301 (5) Å
β = 105.816 (3)°
V = 1654.86 (14) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.73 mm^{-1}
T = 100.0 (1) K
0.45 × 0.12 × 0.10 mm

Data collection

Bruker SMART APEX II CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.734, T_{max} = 0.930
32385 measured reflections
4319 independent reflections
3643 reflections with $I > 2\sigma(I)$
R_{int} = 0.051

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.130
S = 1.12
4319 reflections
236 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.51 e Å^{-3}
$\Delta\rho_{min}$ = −0.60 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2A···O1^{i}	0.82	2.25	2.867 (3)	132
O3A—H3A···Cl1^{ii}	0.82	2.81	3.435 (3)	135
O3A—H3A···Cl2^{ii}	0.82	2.66	3.371 (4)	146
C15—H15A···O2	0.93	2.34	2.733 (3)	105

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2005); program(s) used to solve structure: *SHELXTL* (Sheldrick, 1998); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2402).

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supplementary materials

Acta Cryst. (2007). E**63**, o3385 [**doi:10.1107/S1600536807031509**]

4,5,6,7-Tetrachloro-3-(cyclohepta-1,3,6-trien-1-yl)-3-hydroxy-2-(2-hydroxyethyl)-2,3-dihydro-1*H*-isoindol-1-one

H.-K. Fun, J. B.-J. Teh, Y.-M. Shen and J.-H. Xu

Comment

The construction of medium and large heterocyclic ring systems has constantly been an important task in organic synthesis (Evans & Holmes, 1991; Griesbeck *et al.*, 1996; Illuminati & Mandolini, 1981). In continuation of our recent work on a new strategy for the synthesis of medium to large ring compounds based on photoinduced electron transfer (PET) reactions of N-(ω-hydroxyalkyl)-4,5,6,7- tetrachlorophthalimide (TCP) with electron rich alkenes, we studied the photoinduced reaction of *N*-(2-hydroxyethyl)-4,5,6,7- tetrachlorophthalimide (TCP) with cycloheptatriene and obtained the title compound. We report here the crystal structure of the title compound which is determined to show its steric structure (Xue *et al.*, 2000).

Bond lengths and angles are in normal ranges (Allen *et al.*, 1987) and are comparable to those in a related structure (Fun *et al.*, 2007). The isoindole unit (C1—C8/N1) is essentially planar, with a maximum deviation of 0.066 (2) Å for atom C1. The seven-membered ring adopts a boat conformation.

Intramolecular C15—H15A···O2 interaction generates an S(5) ring motif (Fig. 1) (Bernstein *et al.*, 1995). The crystal structure is stabilized by O—H···O and O—H···Cl (Fig. 2 and Table 1) interactions. These interactions link the molecules into a two-dimensional network parallel to the (0 1 0) plane. The relatively short distance [2.980 (2) Å] between atoms Cl1 and O1($-1-x, -y, 2-z$) indicates the presence of intermolecular Cl···O interactions, which contribute to further stabilization of the crystal structure.

Experimental

The title compound was synthesized by a photo-induced reaction between *N*-(2-hydroxyethyl)-4,5,6,7-tetrachlorophthalimide (0.025 *M*) and excess cycloheptariene in benzene (120 ml). The title compound was isolated using silica gel column chromatography with petroleum ether-ethyl acetate as eluent. Single crystals suitable for X-ray diffraction analysis were obtained by slow evaporation of an ethanol solution.

Refinement

The ratio of the refined occupancies for the major and minor components of the disordered hydroxyl O atoms, O3A and O3B, are 0.509 (5):0.491 (5). H atoms were positioned geometrically and refined using a riding model with O—H = 0.82 Å and C—H = 0.93–0.97 Å, and with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(O).

Figures

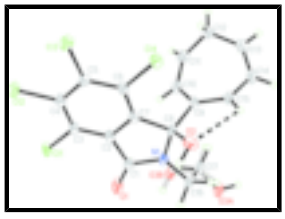

Fig. 1. The molecular structure of the title compound, showing 50% probability displacement ellipsoids and the atomic numbering. Both disorder components are shown. The hydrogen bond is shown as a dashed line.

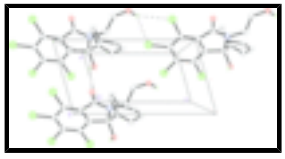

Fig. 2. The crystal packing of the major component, viewed down the *b* axis. For the minor component, the O—H···Cl hydrogen bonds are absent. H atoms not involved in hydrogen bonding (dashed lines) have been omitted.

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Crystal data

$C_{17}H_{13}Cl_4NO_3$	F_{000} = 856
M_r = 421.08	D_x = 1.690 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 9862 reflections
a = 5.7285 (3) Å	θ = 1.5–28.8º
b = 27.9820 (12) Å	μ = 0.73 mm^{-1}
c = 10.7301 (5) Å	T = 100.0 (1) K
β = 105.816 (3)º	Needle, colourless
V = 1654.86 (14) Å^3	0.45 × 0.12 × 0.10 mm
Z = 4	

Data collection

Bruker SMART APEXII CCD area-detector diffractometer	4319 independent reflections
Radiation source: fine-focus sealed tube	3643 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.051
Detector resolution: 8.33 pixels mm^{-1}	θ_{max} = 28.8º
T = 100.0(1) K	θ_{min} = 1.5º
ω scans	h = −7→7
Absorption correction: multi-scan (SADABS; Bruker, 2005)	k = −37→37
T_{min} = 0.734, T_{max} = 0.930	l = −14→14
32385 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.047$

$wR(F^2) = 0.130$

$S = 1.12$

4319 reflections

236 parameters

Primary atom site location: structure-invariant direct methods

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0699P)^2 + 0.7172P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.001$

$\Delta\rho_{max} = 0.51$ e Å^{-3}

$\Delta\rho_{min} = -0.60$ e Å^{-3}

Extinction correction: none

Special details

Experimental. The data was collected with the Oxford Cyrosystem Cobra low-temperature attachment.

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 $F^2 > 2$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}	Occ. (<1)
Cl1	−0.29215 (10)	0.03836 (2)	1.11550 (5)	0.02248 (15)	
Cl2	0.04401 (11)	0.10146 (2)	1.33363 (5)	0.02604 (16)	
Cl3	0.44031 (11)	0.16567 (2)	1.27276 (5)	0.02525 (15)	
Cl4	0.48531 (11)	0.17301 (2)	0.98860 (6)	0.02581 (16)	
O1	−0.2907 (3)	0.01311 (7)	0.83031 (16)	0.0304 (4)	
O2	0.3526 (3)	0.08766 (6)	0.77716 (18)	0.0269 (4)	
H2A	0.3809	0.0603	0.8045	0.040*	
O3A	−0.4124 (7)	0.04349 (13)	0.4118 (3)	0.0292 (10)	0.509 (5)
H3A	−0.3513	0.0577	0.3617	0.044*	0.509 (5)
O3B	−0.5578 (6)	0.05223 (13)	0.5737 (3)	0.0245 (10)	0.491 (5)
H3B	−0.5516	0.0237	0.5919	0.037*	0.491 (5)
N1	−0.0585 (3)	0.06401 (6)	0.74676 (17)	0.0174 (4)	
C1	−0.1487 (4)	0.04629 (8)	0.8422 (2)	0.0183 (4)	
C2	−0.0356 (4)	0.07528 (8)	0.9597 (2)	0.0175 (4)	
C3	−0.0708 (4)	0.07389 (8)	1.0830 (2)	0.0183 (4)	
C4	0.0766 (4)	0.10265 (8)	1.1789 (2)	0.0191 (4)	
C5	0.2515 (4)	0.13256 (8)	1.1510 (2)	0.0188 (4)	
C6	0.2753 (4)	0.13497 (8)	1.0250 (2)	0.0190 (4)	
C7	0.1311 (4)	0.10621 (7)	0.9313 (2)	0.0166 (4)	
C8	0.1250 (4)	0.10192 (8)	0.7885 (2)	0.0172 (4)	
C9	0.0402 (4)	0.14778 (8)	0.7125 (2)	0.0173 (4)	

C10	−0.1781 (4)	0.16913 (8)	0.7316 (2)	0.0210 (5)	
H10A	−0.2893	0.1488	0.7534	0.025*	
C11	−0.2327 (5)	0.21585 (9)	0.7204 (2)	0.0250 (5)	
H11A	−0.3834	0.2257	0.7280	0.030*	
C12	−0.0631 (5)	0.25245 (8)	0.6965 (2)	0.0270 (5)	
H12A	−0.1351	0.2839	0.6960	0.032*	
H12B	0.0857	0.2516	0.7664	0.032*	
C13	−0.0071 (6)	0.24467 (9)	0.5749 (3)	0.0376 (7)	
H13A	−0.0303	0.2702	0.5174	0.045*	
C14	0.0752 (5)	0.20388 (9)	0.5379 (2)	0.0312 (6)	
H14A	0.0825	0.2011	0.4526	0.037*	
C15	0.1538 (4)	0.16358 (8)	0.6247 (2)	0.0209 (5)	
H15A	0.2927	0.1474	0.6196	0.025*	
C16	−0.1193 (4)	0.04355 (8)	0.6172 (2)	0.0206 (5)	
H16A	−0.1414	0.0093	0.6232	0.025*	
H16B	0.0149	0.0487	0.5798	0.025*	
C17	−0.3483 (5)	0.06508 (10)	0.5283 (2)	0.0273 (5)	
H17A	−0.4799	0.0622	0.5687	0.033*	0.509 (5)
H17B	−0.3219	0.0988	0.5166	0.033*	0.509 (5)
H17C	−0.3703	0.0535	0.4417	0.033*	0.491 (5)
H17D	−0.3330	0.0992	0.5271	0.033*	0.491 (5)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0218 (3)	0.0280 (3)	0.0205 (3)	−0.0060 (2)	0.0105 (2)	0.00298 (19)
Cl2	0.0296 (3)	0.0344 (3)	0.0164 (3)	−0.0046 (3)	0.0102 (2)	0.0011 (2)
Cl3	0.0235 (3)	0.0305 (3)	0.0224 (3)	−0.0057 (2)	0.0072 (2)	−0.0047 (2)
Cl4	0.0251 (3)	0.0285 (3)	0.0286 (3)	−0.0099 (2)	0.0152 (3)	−0.0029 (2)
O1	0.0278 (10)	0.0425 (10)	0.0237 (8)	−0.0179 (8)	0.0115 (8)	−0.0051 (7)
O2	0.0189 (8)	0.0211 (8)	0.0478 (10)	0.0030 (7)	0.0215 (8)	0.0033 (7)
O3A	0.032 (2)	0.038 (2)	0.0192 (16)	−0.0147 (16)	0.0093 (15)	−0.0078 (13)
O3B	0.0146 (17)	0.039 (2)	0.0222 (17)	0.0011 (15)	0.0082 (14)	−0.0021 (14)
N1	0.0166 (9)	0.0211 (9)	0.0170 (8)	0.0003 (7)	0.0090 (8)	0.0002 (6)
C1	0.0141 (10)	0.0233 (10)	0.0189 (10)	0.0016 (9)	0.0071 (9)	0.0017 (8)
C2	0.0141 (10)	0.0218 (10)	0.0179 (9)	0.0020 (9)	0.0065 (9)	0.0038 (8)
C3	0.0157 (11)	0.0223 (10)	0.0186 (10)	0.0000 (9)	0.0077 (9)	0.0035 (8)
C4	0.0181 (11)	0.0233 (10)	0.0183 (10)	0.0029 (9)	0.0087 (9)	0.0032 (8)
C5	0.0180 (11)	0.0208 (10)	0.0189 (10)	0.0009 (9)	0.0072 (9)	−0.0011 (8)
C6	0.0167 (11)	0.0196 (10)	0.0233 (10)	−0.0004 (9)	0.0099 (9)	0.0022 (8)
C7	0.0132 (10)	0.0191 (10)	0.0188 (10)	0.0029 (8)	0.0065 (9)	0.0037 (7)
C8	0.0162 (11)	0.0207 (10)	0.0185 (9)	0.0024 (9)	0.0111 (9)	0.0009 (8)
C9	0.0171 (11)	0.0201 (10)	0.0163 (9)	0.0003 (9)	0.0070 (9)	0.0012 (8)
C10	0.0194 (12)	0.0252 (11)	0.0196 (10)	0.0022 (9)	0.0074 (9)	0.0024 (8)
C11	0.0237 (12)	0.0257 (11)	0.0281 (12)	0.0049 (10)	0.0112 (10)	0.0008 (9)
C12	0.0316 (14)	0.0210 (11)	0.0314 (12)	0.0031 (10)	0.0139 (11)	0.0019 (9)
C13	0.056 (2)	0.0247 (12)	0.0430 (15)	0.0027 (13)	0.0313 (15)	0.0060 (11)
C14	0.0457 (17)	0.0321 (13)	0.0223 (11)	0.0055 (12)	0.0201 (12)	0.0068 (10)

C15	0.0226 (12)	0.0233 (11)	0.0206 (10)	0.0023 (9)	0.0125 (10)	0.0010 (8)
C16	0.0188 (11)	0.0268 (11)	0.0186 (10)	−0.0010 (9)	0.0093 (9)	−0.0033 (8)
C17	0.0204 (12)	0.0454 (15)	0.0192 (10)	0.0022 (11)	0.0106 (10)	−0.0003 (10)

Geometric parameters (Å, °)

Cl1—C3	1.720 (2)	C8—C9	1.527 (3)
Cl2—C4	1.721 (2)	C9—C15	1.357 (3)
Cl3—C5	1.722 (2)	C9—C10	1.450 (3)
Cl4—C6	1.728 (2)	C10—C11	1.342 (3)
O1—C1	1.218 (3)	C10—H10A	0.93
O2—C8	1.400 (3)	C11—C12	1.481 (4)
O2—H2A	0.82	C11—H11A	0.93
O3A—C17	1.346 (4)	C12—C13	1.443 (4)
O3A—H3A	0.82	C12—H12A	0.97
O3A—H17C	0.4437	C12—H12B	0.97
O3B—C17	1.458 (4)	C13—C14	1.336 (4)
O3B—H3B	0.82	C13—H13A	0.93
N1—C1	1.360 (3)	C14—C15	1.453 (3)
N1—C16	1.455 (3)	C14—H14A	0.93
N1—C8	1.475 (3)	C15—H15A	0.93
C1—C2	1.491 (3)	C16—C17	1.520 (3)
C2—C7	1.383 (3)	C16—H16A	0.97
C2—C3	1.392 (3)	C16—H16B	0.97
C3—C4	1.395 (3)	C17—H17A	0.97
C4—C5	1.399 (3)	C17—H17B	0.97
C5—C6	1.398 (3)	C17—H17C	0.96
C6—C7	1.374 (3)	C17—H17D	0.96
C7—C8	1.527 (3)		
C8—O2—H2A	109.5	C10—C11—H11A	118.6
C17—O3A—H3A	109.5	C12—C11—H11A	118.6
H3A—O3A—H17C	85.6	C13—C12—C11	111.7 (2)
C17—O3B—H3B	109.5	C13—C12—H12A	109.3
C1—N1—C16	122.32 (19)	C11—C12—H12A	109.3
C1—N1—C8	114.78 (18)	C13—C12—H12B	109.3
C16—N1—C8	122.59 (18)	C11—C12—H12B	109.3
O1—C1—N1	125.4 (2)	H12A—C12—H12B	107.9
O1—C1—C2	128.9 (2)	C14—C13—C12	125.5 (2)
N1—C1—C2	105.76 (19)	C14—C13—H13A	117.2
C7—C2—C3	121.0 (2)	C12—C13—H13A	117.2
C7—C2—C1	108.73 (18)	C13—C14—C15	123.0 (2)
C3—C2—C1	130.3 (2)	C13—C14—H14A	118.5
C2—C3—C4	118.0 (2)	C15—C14—H14A	118.5
C2—C3—Cl1	120.99 (17)	C9—C15—C14	125.0 (2)
C4—C3—Cl1	121.00 (16)	C9—C15—H15A	117.5
C3—C4—C5	120.8 (2)	C14—C15—H15A	117.5
C3—C4—Cl2	119.84 (17)	N1—C16—C17	112.61 (19)
C5—C4—Cl2	119.36 (17)	N1—C16—H16A	109.1
C6—C5—C4	120.0 (2)	C17—C16—H16A	109.1

C6—C5—Cl3	120.09 (17)	N1—C16—H16B	109.1
C4—C5—Cl3	119.88 (16)	C17—C16—H16B	109.1
C7—C6—C5	118.8 (2)	H16A—C16—H16B	107.8
C7—C6—Cl4	120.79 (17)	O3A—C17—O3B	99.1 (3)
C5—C6—Cl4	120.39 (17)	O3A—C17—C16	112.0 (3)
C6—C7—C2	121.2 (2)	O3B—C17—C16	109.9 (2)
C6—C7—C8	128.67 (19)	O3A—C17—H17A	109.2
C2—C7—C8	110.09 (19)	C16—C17—H17A	109.2
O2—C8—N1	111.84 (17)	O3A—C17—H17B	109.2
O2—C8—C7	110.02 (18)	O3B—C17—H17B	117.1
N1—C8—C7	100.43 (16)	C16—C17—H17B	109.2
O2—C8—C9	111.15 (18)	H17A—C17—H17B	107.9
N1—C8—C9	110.21 (18)	O3B—C17—H17C	109.7
C7—C8—C9	112.76 (17)	C16—C17—H17C	109.7
C15—C9—C10	124.0 (2)	H17A—C17—H17C	119.4
C15—C9—C8	120.1 (2)	H17B—C17—H17C	100.8
C10—C9—C8	115.55 (18)	O3A—C17—H17D	115.9
C11—C10—C9	125.3 (2)	O3B—C17—H17D	109.7
C11—C10—H10A	117.4	C16—C17—H17D	109.7
C9—C10—H10A	117.4	H17A—C17—H17D	100.1
C10—C11—C12	122.8 (2)	H17C—C17—H17D	108.2
C16—N1—C1—O1	−1.8 (4)	C1—N1—C8—O2	115.3 (2)
C8—N1—C1—O1	−175.5 (2)	C16—N1—C8—O2	−58.4 (3)
C16—N1—C1—C2	177.46 (19)	C1—N1—C8—C7	−1.4 (2)
C8—N1—C1—C2	3.8 (2)	C16—N1—C8—C7	−175.08 (18)
O1—C1—C2—C7	174.5 (2)	C1—N1—C8—C9	−120.6 (2)
N1—C1—C2—C7	−4.8 (2)	C16—N1—C8—C9	65.8 (2)
O1—C1—C2—C3	−3.8 (4)	C6—C7—C8—O2	59.6 (3)
N1—C1—C2—C3	177.0 (2)	C2—C7—C8—O2	−119.8 (2)
C7—C2—C3—C4	−3.6 (3)	C6—C7—C8—N1	177.6 (2)
C1—C2—C3—C4	174.5 (2)	C2—C7—C8—N1	−1.8 (2)
C7—C2—C3—Cl1	175.60 (17)	C6—C7—C8—C9	−65.1 (3)
C1—C2—C3—Cl1	−6.3 (3)	C2—C7—C8—C9	115.5 (2)
C2—C3—C4—C5	1.1 (3)	O2—C8—C9—C15	13.9 (3)
Cl1—C3—C4—C5	−178.07 (17)	N1—C8—C9—C15	−110.7 (2)
C2—C3—C4—Cl2	−178.86 (17)	C7—C8—C9—C15	138.0 (2)
Cl1—C3—C4—Cl2	2.0 (3)	O2—C8—C9—C10	−172.13 (19)
C3—C4—C5—C6	1.9 (3)	N1—C8—C9—C10	63.3 (2)
Cl2—C4—C5—C6	−178.11 (17)	C7—C8—C9—C10	−48.0 (3)
C3—C4—C5—Cl3	−177.09 (17)	C15—C9—C10—C11	−34.4 (4)
Cl2—C4—C5—Cl3	2.9 (3)	C8—C9—C10—C11	151.9 (2)
C4—C5—C6—C7	−2.5 (3)	C9—C10—C11—C12	−5.0 (4)
Cl3—C5—C6—C7	176.50 (17)	C10—C11—C12—C13	61.7 (3)
C4—C5—C6—Cl4	178.26 (17)	C11—C12—C13—C14	−53.2 (4)
Cl3—C5—C6—Cl4	−2.7 (3)	C12—C13—C14—C15	−9.5 (5)
C5—C6—C7—C2	0.1 (3)	C10—C9—C15—C14	0.2 (4)
Cl4—C6—C7—C2	179.29 (17)	C8—C9—C15—C14	173.6 (2)
C5—C6—C7—C8	−179.2 (2)	C13—C14—C15—C9	41.3 (4)
Cl4—C6—C7—C8	0.0 (3)	C1—N1—C16—C17	87.9 (3)

C3—C2—C7—C6	3.1 (3)	C8—N1—C16—C17	−98.9 (2)
C1—C2—C7—C6	−175.4 (2)	N1—C16—C17—O3A	−175.5 (2)
C3—C2—C7—C8	−177.52 (19)	N1—C16—C17—O3B	−66.3 (3)
C1—C2—C7—C8	4.0 (2)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2A···O1^{i}	0.82	2.25	2.867 (3)	132
O3A—H3A···Cl1^{ii}	0.82	2.81	3.435 (3)	135
O3A—H3A···Cl2^{ii}	0.82	2.66	3.371 (4)	146
C15—H15A···O2	0.93	2.34	2.733 (3)	105

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

Fig. 1

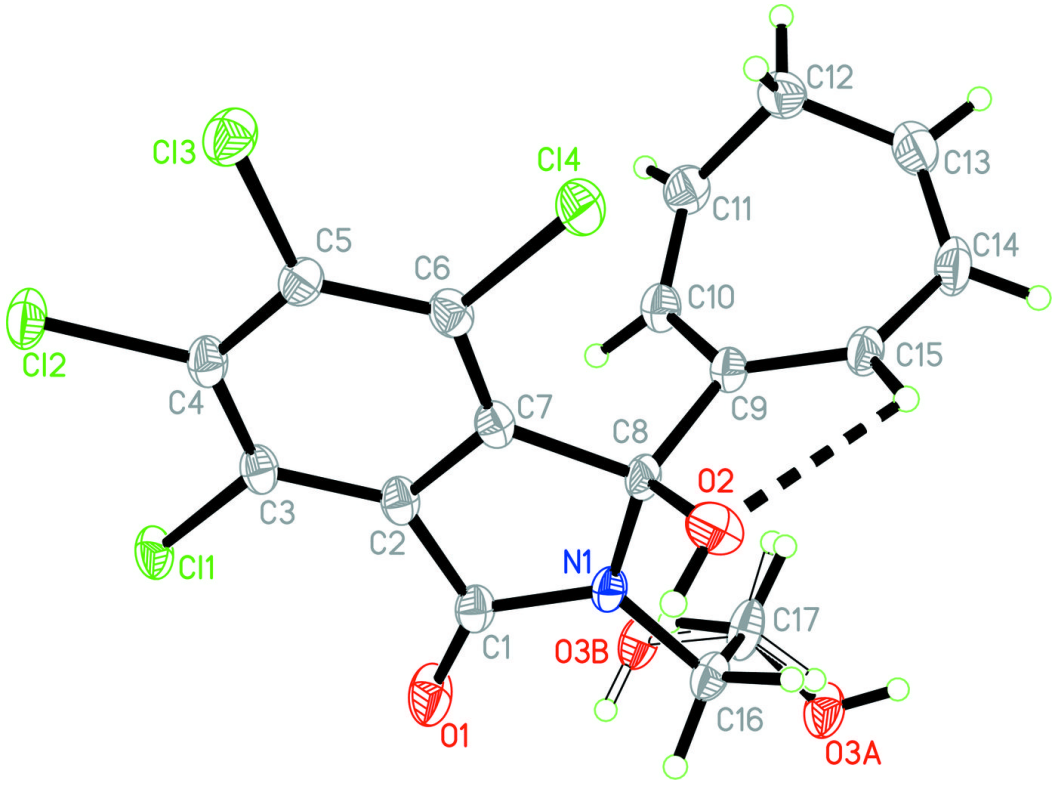
C12
C13
C14
C11
C10
C15
C9
C8
C7
C6
C5
C4
C3
C2
C1
Cl3
Cl4
Cl2
Cl1
O2
N1
O3B
O3A
C17
C16
O1

Fig. 2