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1,5-Bis(2,6-dichlorophenyl)-3-[(1*H*-1,2,4-triazol-1-yl)methyl]penta-1,4-dien-3-ol

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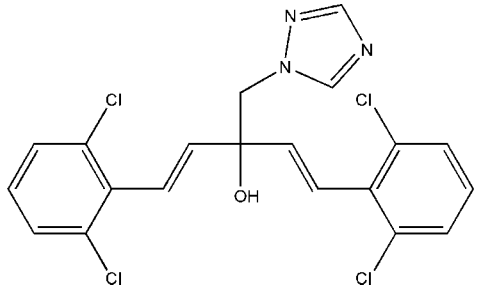
Key indicators: single-crystal X-ray study; T = 153 K; mean σ(C–C) = 0.003 Å; R factor = 0.031; wR factor = 0.085; data-to-parameter ratio = 13.4.

The title compound, $C_{20}H_{15}Cl_4N_3O$, was prepared by the reaction of 2,2-bis(2,6-dichlorostyryl)oxirane and 1,2,4-triazole. In the crystal structure, molecules assemble along the b axis, forming helical suprastructures, which further assemble along the c axis, forming two-dimensional layer structures.

Related literature

For related literature, see: Graham & Jorg (1985); Massa *et al.* (1992); Rong *et al.* (2006).



Experimental

Crystal data

$C_{20}H_{15}Cl_4N_3O$
M_r = 455.15
Monoclinic, $P2_1/c$
a = 8.3413 (17) Å
b = 10.652 (2) Å
c = 22.229 (4) Å
β = 94.32 (3)°
V = 1969.5 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.62 mm^{-1}
T = 153 (2) K
0.32 × 0.22 × 0.16 mm

Data collection

Rigaku RAXIS-RAPID IP area-detector diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi 1995)
T_{min} = 0.827, T_{max} = 0.908
15134 measured reflections
3470 independent reflections
2901 reflections with $I > 2\sigma(I)$
R_{int} = 0.031

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.085
S = 1.06
3470 reflections
258 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1A···N3^{i}	0.74 (2)	2.22 (2)	2.940 (2)	163 (2)

Symmetry code: (i) $-x+2, -y, -z+1$.

Data collection: *RAPID-AUTO* (Rigaku 2004); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2001); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG2350).

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supplementary materials

Acta Cryst. (2007). E**63**, o4848 [**doi:10.1107/S1600536807058898**]

1,5-Bis(2,6-dichlorophenyl)-3-[(1*H*-1,2,4-triazol-1-yl)methyl]penta-1,4-dien-3-ol

L.-Z. Xu, G.-S. Zhang, X. Yi, G.-W. An and Z.-J. Xu

Comment

Derivatives of 1,2,4-triazole are known to exhibit diverse applications in the fields of medicine, agriculture and industry. Among the agriculture profiles of various 1,2,4-triazole and its derivatives, their fungicidal, bactericidal, pesticidal and plant growth properties (Massa *et al.*, 1992) seem to be the most widely documented. For these reasons, the structures of substituted 1,2,4-triazole have been a subject of interest in our laboratory. The crystal structure of the title compound is presented here.

The bond lengths and angles are normal for this type of compound (Rong *et al.*, 2006). The dihedral angles formed by phenyl ring (C1 - C6) and phenyl ring (C13 –C18) with plane (N1/N2/N3/C19/C20) are 34.20 (2) and 10.10 (2)°, respectively. The dihedral angle between the benzene rings is 24.41 (3)°. The molecules assemble to form helical superstructures along the *b* axis. The helic pitch is 10.65 (2) Å. The right-handed and left-handed helix associate through weak hydrogen bonds, which further assemble along *c* axis to form two-dimensional layer structure through O—H···N hydrogen bonds.

Experimental

A mixture of 1,2,4-triazole 0.90 g (0.013 mol), 2,2-bis(2,6-dichlorostyryl)oxirane 3.86 g (0.01 mol) dissolved in DMF and powdered potassium carbonate 0.1 g was stirred vigorously at gentle reflux for 2 h (Graham *et al.*, 1985). The reaction mixture was cooled, then concentrated by removing the solvent under reduced pressure·The residue was taken up in water. The solid residue was then recrystallized from ethanol to give 3-((1*H*-1,2,4-triazol-1-yl)methyl)-1,5-bis(2,6-dichlorophenyl) penta-1,4-dien-3-ol 3.64 g(yield 80%). Single crystals suitable for X-ray measurement were obtained by recrystallization from methanol at room temperature.

Refinement

All H atoms were found on difference maps. The hydroxyl H atoms were refined freely, giving an O—H bond distance of 0.74 Å. The remaining H atoms were placed in calculated positions, with C—H = 0.95 or 0.99 Å, and included in the final cycles of refinement using a riding model, with U_{iso}(H) = 1.2 times U_{eq}(C).

Figures

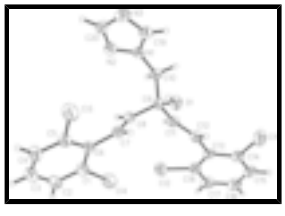

Fig. 1. View of the title compound (I), with displacement ellipsoids drawn at the 35% probability level.

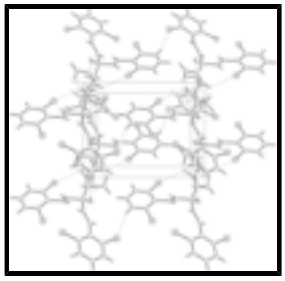

Fig. 2. A packing diagram of the molecule of the title compound, view down *b* axis. Hydrogen bonds are shown as dashed lines.

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Crystal data

$C_{20}H_{15}Cl_4N_3O$	F_{000} = 928
M_r = 455.15	D_x = 1.535 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 1494 reflections
a = 8.3413 (17) Å	θ = 2.6–26.4º
b = 10.652 (2) Å	μ = 0.62 mm^{-1}
c = 22.229 (4) Å	T = 153 (2) K
β = 94.32 (3)º	Block, colorless
V = 1969.5 (7) Å^3	0.32 × 0.22 × 0.16 mm
Z = 4	

Data collection

Rigaku RAXIS RAPID IP area-detector diffractometer	3470 independent reflections
Radiation source: Rotating Anode	2901 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.031
T = 153(2) K	θ_{max} = 25.0º
ω Oscillation scans	θ_{min} = 3.1º
Absorption correction: multi-scan (ABSCOR; Higashi 1995)	h = −9→9
T_{min} = 0.827, T_{max} = 0.908	k = −12→11
15134 measured reflections	l = −26→26

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)]$ = 0.031	$w = 1/[\sigma^2(F_o^2) + (0.0359P)^2 + 0.8502P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.085	$(\Delta/\sigma)_{max}$ = 0.001
S = 1.06	$\Delta\rho_{max}$ = 0.27 e Å^{-3}

3470 reflections	$\Delta\rho_{min} = -0.22$ e Å^{-3}
258 parameters	Extinction correction: SHELXL, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0048 (6)
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 $F^2 > 2\text{sigma}(F^2)$ 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	0.43666 (7)	0.42402 (6)	0.34867 (3)	0.06239 (19)
Cl2	0.33568 (7)	0.22308 (5)	0.23550 (3)	0.05817 (18)
Cl3	0.85225 (8)	0.35813 (5)	0.54500 (3)	0.0637 (2)
Cl1	0.23987 (7)	−0.25254 (6)	0.31663 (3)	0.0666 (2)
O1	0.64236 (17)	−0.00926 (13)	0.42224 (7)	0.0441 (4)
N1	0.98450 (18)	0.03373 (14)	0.38889 (7)	0.0387 (4)
C13	0.2879 (2)	−0.01739 (17)	0.27484 (8)	0.0351 (4)
C6	0.6561 (2)	0.39721 (17)	0.44453 (8)	0.0348 (4)
N2	1.0809 (2)	0.13526 (15)	0.38301 (8)	0.0473 (4)
C10	0.8402 (2)	0.01560 (19)	0.34845 (9)	0.0433 (5)
H10A	0.8277	−0.0752	0.3397	0.052*
H10B	0.8554	0.0587	0.3098	0.052*
C9	0.6840 (2)	0.06435 (16)	0.37317 (8)	0.0348 (4)
C11	0.5554 (2)	0.05100 (18)	0.32121 (8)	0.0384 (4)
H11A	0.5765	0.0882	0.2838	0.046*
C15	0.0685 (2)	−0.1425 (2)	0.22533 (9)	0.0471 (5)
H15A	0.0088	−0.2185	0.2234	0.057*
N3	1.1824 (2)	0.00913 (18)	0.45797 (8)	0.0521 (5)
C12	0.4179 (2)	−0.00754 (18)	0.32389 (8)	0.0383 (4)
H12A	0.3998	−0.0477	0.3609	0.046*
C8	0.6932 (2)	0.20331 (16)	0.38717 (8)	0.0352 (4)
H8A	0.7318	0.2559	0.3569	0.042*
C14	0.1950 (2)	−0.12640 (19)	0.26875 (8)	0.0400 (4)
C4	0.7604 (3)	0.58210 (19)	0.50010 (9)	0.0500 (5)
H4A	0.8260	0.6162	0.5329	0.060*
C1	0.5691 (2)	0.48093 (18)	0.40644 (9)	0.0414 (4)
C5	0.7486 (2)	0.45377 (18)	0.49228 (8)	0.0397 (4)

C17	0.1171 (2)	0.0629 (2)	0.18888 (9)	0.0495 (5)
H17A	0.0916	0.1289	0.1610	0.059*
C20	1.1960 (2)	0.1150 (2)	0.42536 (9)	0.0475 (5)
H20A	1.2836	0.1714	0.4327	0.057*
C18	0.2413 (2)	0.07738 (18)	0.23329 (9)	0.0404 (4)
C7	0.6534 (2)	0.25908 (17)	0.43680 (8)	0.0367 (4)
H7A	0.6215	0.2085	0.4690	0.044*
C19	1.0475 (2)	−0.0394 (2)	0.43300 (9)	0.0477 (5)
H19A	1.0018	−0.1163	0.4450	0.057*
C2	0.5793 (3)	0.60988 (19)	0.41337 (9)	0.0473 (5)
H2B	0.5191	0.6636	0.3860	0.057*
C16	0.0304 (2)	−0.0475 (2)	0.18522 (9)	0.0525 (6)
H16A	−0.0554	−0.0576	0.1550	0.063*
C3	0.6762 (3)	0.65986 (19)	0.45980 (10)	0.0508 (5)
H3B	0.6852	0.7484	0.4641	0.061*
H1A	0.686 (3)	0.006 (2)	0.4516 (11)	0.050 (7)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl4	0.0641 (4)	0.0592 (3)	0.0593 (3)	0.0088 (3)	−0.0255 (3)	−0.0059 (3)
Cl2	0.0587 (3)	0.0427 (3)	0.0695 (4)	0.0006 (2)	−0.0191 (3)	0.0066 (2)
Cl3	0.0799 (4)	0.0533 (3)	0.0535 (3)	0.0072 (3)	−0.0249 (3)	0.0025 (3)
Cl1	0.0618 (4)	0.0589 (4)	0.0756 (4)	−0.0161 (3)	−0.0185 (3)	0.0215 (3)
O1	0.0496 (8)	0.0393 (7)	0.0408 (8)	−0.0077 (6)	−0.0145 (7)	0.0034 (6)
N1	0.0343 (8)	0.0369 (8)	0.0433 (9)	0.0072 (7)	−0.0084 (7)	−0.0077 (7)
C13	0.0291 (9)	0.0435 (10)	0.0321 (9)	0.0039 (8)	−0.0022 (7)	−0.0061 (8)
C6	0.0360 (9)	0.0345 (9)	0.0342 (9)	0.0006 (8)	0.0053 (8)	−0.0016 (8)
N2	0.0450 (9)	0.0413 (9)	0.0542 (10)	0.0001 (8)	−0.0055 (8)	−0.0035 (8)
C10	0.0387 (10)	0.0443 (11)	0.0445 (11)	0.0073 (8)	−0.0133 (9)	−0.0144 (9)
C9	0.0341 (9)	0.0330 (9)	0.0355 (9)	0.0016 (7)	−0.0090 (8)	−0.0011 (7)
C11	0.0366 (10)	0.0428 (10)	0.0345 (10)	0.0046 (8)	−0.0067 (8)	−0.0006 (8)
C15	0.0343 (10)	0.0568 (13)	0.0492 (12)	−0.0051 (9)	−0.0040 (9)	−0.0114 (10)
N3	0.0391 (9)	0.0672 (12)	0.0482 (10)	0.0071 (8)	−0.0092 (8)	−0.0006 (9)
C12	0.0386 (10)	0.0405 (10)	0.0344 (10)	0.0043 (8)	−0.0062 (8)	−0.0037 (8)
C8	0.0326 (9)	0.0339 (9)	0.0385 (10)	0.0019 (8)	−0.0004 (8)	0.0014 (8)
C14	0.0334 (9)	0.0475 (11)	0.0385 (10)	0.0024 (8)	−0.0015 (8)	−0.0016 (8)
C4	0.0618 (13)	0.0412 (11)	0.0460 (12)	−0.0055 (10)	−0.0027 (10)	−0.0079 (9)
C1	0.0428 (10)	0.0421 (11)	0.0385 (10)	0.0021 (8)	−0.0013 (8)	−0.0025 (8)
C5	0.0427 (10)	0.0385 (10)	0.0372 (10)	0.0022 (8)	−0.0009 (8)	0.0023 (8)
C17	0.0425 (11)	0.0588 (13)	0.0447 (11)	0.0090 (10)	−0.0127 (9)	0.0024 (10)
C20	0.0379 (10)	0.0524 (12)	0.0513 (12)	−0.0012 (9)	−0.0039 (9)	−0.0129 (10)
C18	0.0358 (10)	0.0420 (10)	0.0422 (10)	0.0034 (8)	−0.0050 (8)	−0.0037 (9)
C7	0.0371 (9)	0.0347 (9)	0.0378 (10)	0.0002 (8)	−0.0003 (8)	0.0016 (8)
C19	0.0417 (11)	0.0462 (11)	0.0536 (12)	0.0072 (9)	−0.0062 (10)	0.0034 (10)
C2	0.0556 (12)	0.0396 (11)	0.0464 (11)	0.0093 (9)	0.0027 (10)	0.0066 (9)
C16	0.0374 (11)	0.0726 (15)	0.0447 (12)	0.0037 (10)	−0.0147 (9)	−0.0085 (11)
C3	0.0669 (14)	0.0325 (10)	0.0535 (13)	−0.0003 (10)	0.0083 (11)	−0.0021 (9)

Geometric parameters (Å, °)

Cl4—C1	1.739 (2)	C15—C16	1.370 (3)
Cl2—C18	1.739 (2)	C15—C14	1.386 (3)
Cl3—C5	1.7341 (19)	C15—H15A	0.9500
Cl1—C14	1.737 (2)	N3—C19	1.322 (3)
O1—C9	1.408 (2)	N3—C20	1.350 (3)
O1—H1A	0.74 (2)	C12—H12A	0.9500
N1—C19	1.329 (2)	C8—C7	1.317 (3)
N1—N2	1.360 (2)	C8—H8A	0.9500
N1—C10	1.460 (2)	C4—C3	1.374 (3)
C13—C14	1.397 (3)	C4—C5	1.381 (3)
C13—C18	1.403 (3)	C4—H4A	0.9500
C13—C12	1.483 (2)	C1—C2	1.384 (3)
C6—C1	1.395 (3)	C17—C16	1.380 (3)
C6—C5	1.400 (3)	C17—C18	1.385 (3)
C6—C7	1.481 (2)	C17—H17A	0.9500
N2—C20	1.311 (3)	C20—H20A	0.9500
C10—C9	1.542 (3)	C7—H7A	0.9500
C10—H10A	0.9900	C19—H19A	0.9500
C10—H10B	0.9900	C2—C3	1.370 (3)
C9—C8	1.513 (2)	C2—H2B	0.9500
C9—C11	1.523 (2)	C16—H16A	0.9500
C11—C12	1.310 (3)	C3—H3B	0.9500
C11—H11A	0.9500		
C9—O1—H1A	115.4 (19)	C15—C14—C13	123.92 (18)
C19—N1—N2	109.47 (15)	C15—C14—Cl1	116.65 (16)
C19—N1—C10	129.67 (17)	C13—C14—Cl1	119.42 (14)
N2—N1—C10	120.81 (16)	C3—C4—C5	119.11 (19)
C14—C13—C18	114.21 (16)	C3—C4—H4A	120.4
C14—C13—C12	119.99 (16)	C5—C4—H4A	120.4
C18—C13—C12	125.74 (17)	C2—C1—C6	122.84 (18)
C1—C6—C5	114.62 (17)	C2—C1—Cl4	117.28 (15)
C1—C6—C7	124.18 (16)	C6—C1—Cl4	119.86 (15)
C5—C6—C7	121.20 (16)	C4—C5—C6	123.48 (18)
C20—N2—N1	101.93 (16)	C4—C5—Cl3	117.98 (15)
N1—C10—C9	114.57 (15)	C6—C5—Cl3	118.53 (15)
N1—C10—H10A	108.6	C16—C17—C18	119.83 (19)
C9—C10—H10A	108.6	C16—C17—H17A	120.1
N1—C10—H10B	108.6	C18—C17—H17A	120.1
C9—C10—H10B	108.6	N2—C20—N3	115.85 (18)
H10A—C10—H10B	107.6	N2—C20—H20A	122.1
O1—C9—C8	113.39 (15)	N3—C20—H20A	122.1
O1—C9—C11	109.57 (15)	C17—C18—C13	122.98 (18)
C8—C9—C11	105.62 (14)	C17—C18—Cl2	115.59 (15)
O1—C9—C10	110.66 (15)	C13—C18—Cl2	121.41 (14)
C8—C9—C10	111.81 (15)	C8—C7—C6	122.85 (17)
C11—C9—C10	105.33 (15)	C8—C7—H7A	118.6

C12—C11—C9	125.37 (18)	C6—C7—H7A	118.6
C12—C11—H11A	117.3	N3—C19—N1	110.91 (19)
C9—C11—H11A	117.3	N3—C19—H19A	124.5
C16—C15—C14	119.26 (19)	N1—C19—H19A	124.5
C16—C15—H15A	120.4	C3—C2—C1	119.81 (19)
C14—C15—H15A	120.4	C3—C2—H2B	120.1
C19—N3—C20	101.83 (17)	C1—C2—H2B	120.1
C11—C12—C13	126.46 (18)	C15—C16—C17	119.77 (17)
C11—C12—H12A	116.8	C15—C16—H16A	120.1
C13—C12—H12A	116.8	C17—C16—H16A	120.1
C7—C8—C9	126.96 (17)	C2—C3—C4	120.05 (19)
C7—C8—H8A	116.5	C2—C3—H3B	120.0
C9—C8—H8A	116.5	C4—C3—H3B	120.0
C19—N1—N2—C20	−0.5 (2)	C3—C4—C5—C6	0.9 (3)
C10—N1—N2—C20	−178.22 (16)	C3—C4—C5—Cl3	−178.38 (17)
C19—N1—C10—C9	87.3 (2)	C1—C6—C5—C4	−3.0 (3)
N2—N1—C10—C9	−95.5 (2)	C7—C6—C5—C4	177.26 (19)
N1—C10—C9—O1	−68.6 (2)	C1—C6—C5—Cl3	176.25 (14)
N1—C10—C9—C8	58.8 (2)	C7—C6—C5—Cl3	−3.5 (3)
N1—C10—C9—C11	173.04 (16)	N1—N2—C20—N3	0.1 (2)
O1—C9—C11—C12	7.5 (3)	C19—N3—C20—N2	0.3 (2)
C8—C9—C11—C12	−115.0 (2)	C16—C17—C18—C13	1.7 (3)
C10—C9—C11—C12	126.6 (2)	C16—C17—C18—Cl2	−177.19 (17)
C9—C11—C12—C13	177.26 (17)	C14—C13—C18—C17	−1.8 (3)
C14—C13—C12—C11	145.6 (2)	C12—C13—C18—C17	−179.10 (19)
C18—C13—C12—C11	−37.2 (3)	C14—C13—C18—Cl2	177.03 (14)
O1—C9—C8—C7	−6.4 (2)	C12—C13—C18—Cl2	−0.2 (3)
C11—C9—C8—C7	113.6 (2)	C9—C8—C7—C6	−175.63 (16)
C10—C9—C8—C7	−132.37 (19)	C1—C6—C7—C8	57.6 (3)
C16—C15—C14—C13	0.4 (3)	C5—C6—C7—C8	−122.7 (2)
C16—C15—C14—Cl1	−178.21 (16)	C20—N3—C19—N1	−0.7 (2)
C18—C13—C14—C15	0.8 (3)	N2—N1—C19—N3	0.8 (2)
C12—C13—C14—C15	178.21 (18)	C10—N1—C19—N3	178.20 (18)
C18—C13—C14—Cl1	179.34 (14)	C6—C1—C2—C3	−1.0 (3)
C12—C13—C14—Cl1	−3.2 (2)	Cl4—C1—C2—C3	177.09 (17)
C5—C6—C1—C2	3.0 (3)	C14—C15—C16—C17	−0.6 (3)
C7—C6—C1—C2	−177.25 (19)	C18—C17—C16—C15	−0.4 (3)
C5—C6—C1—Cl4	−174.96 (14)	C1—C2—C3—C4	−1.4 (3)
C7—C6—C1—Cl4	4.7 (3)	C5—C4—C3—C2	1.4 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1A···N3^{i}	0.74 (2)	2.22 (2)	2.940 (2)	163 (2)

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

Fig. 1

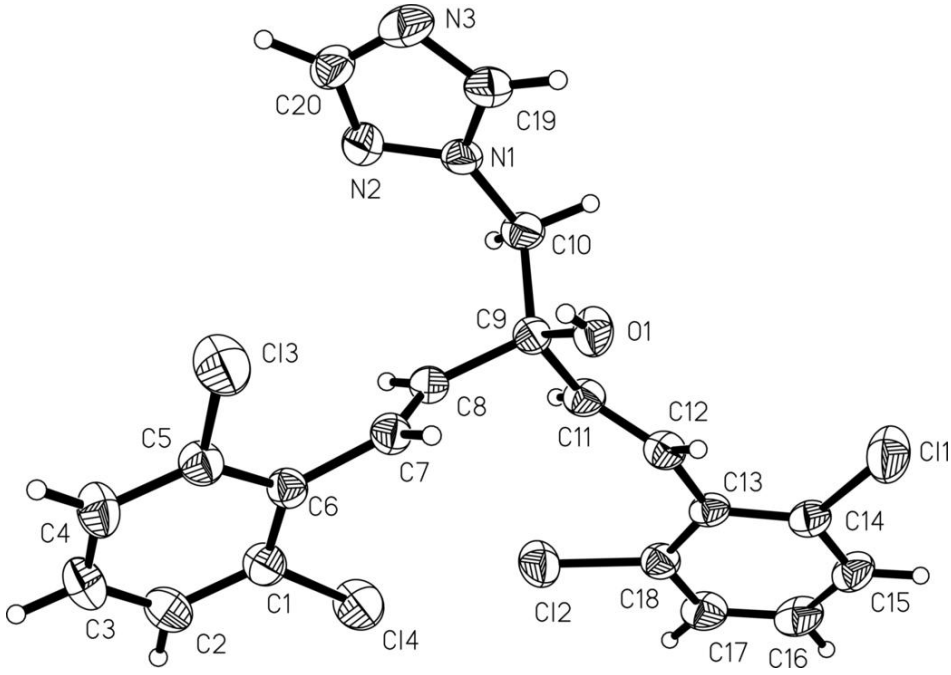
N3
C20
C19
N1
N2
C10
C9
O1
Cl3
C8
C12
C5
C11
Cl1
C7
C13
C6
C14
C4
C18
C15
Cl2
C1
C3
C2
Cl4
C17
C16

Fig. 2