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(*S*)-(+)-2,2′-Bis(2-hydroxy-3-methoxybenzylideneamino)-1,1′-binaphthyl

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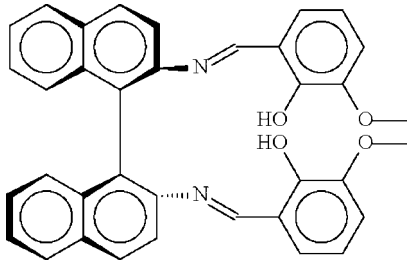
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.006 Å; disorder in main residue; R factor = 0.058; wR factor = 0.203; data-to-parameter ratio = 6.8.

In the chiral title compound, $C_{36}H_{28}N_2O_4$, the two naphthyl systems are twisted by 81.2 (1)° about their linking C—C single bond. The OH group forms an intramolecular hydrogen bond with the imino N acceptor atom. The complete molecule has twofold symmetry and shows extensive disorder of the pendant substituted aromatic ring; the site occupancy ratio is 0.78:0.22.

Related literature

For the crystal structure of the racemic modification of the title compound, see Che *et al.*, 2002; for the opposite enantiomer of the starting material, see: Jones *et al.* (2003). For related literature, see: Suga *et al.* (2003, 2004).



Experimental

Crystal data

$C_{36}H_{28}N_2O_4$
M_r = 552.60
Tetragonal, $P4_12_12$
a = 11.3285 (6) Å
c = 23.837 (1) Å
V = 3059.1 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 295 (2) K
0.38 × 0.31 × 0.28 mm

Data collection

Bruker APEX diffractometer
Absorption correction: none
15298 measured reflections
1629 independent reflections
1190 reflections with $I > 2\sigma(I)$
R_{int} = 0.028

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.203
S = 1.10
1629 reflections
240 parameters
114 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1	0.82	1.86	2.575 (4)	145

Data collection: *SMART* (Bruker, 2003); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2007).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2421).

References

Barbour, L. J. (2001). J. Supramol. Chem. 1, 189–191.
Bruker (2003). *SMART* (Version 6.28a) and *SAINT*. (Version 6.28a). Bruker AXS Inc., Madison, Wisconsin, USA.
Che, C.-M., Kwong, H.-L., Chu, W.-C., Cheung, K.-F., Lee, W.-S., Yu, H.-S., Yeung, C.-T. & Cheung, K.-K. (2002). *Eur. J. Inorg. Chem.* pp. 1456–1463.
Jones, M. D., Almeida Paz, F. A., Davies, J. E. & Johnson, B. F. G. (2003). *Acta Cryst.* E**59**, o910–o912.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Suga, H., Kakehi, A., Ito, S. & Sugimoto, H. (2003). *Bull. Chem. Soc. Jpn*, **76**, 327–334.
Suga, H., Kakehi, A. & Mitsuda, M. (2004). *Bull. Chem. Soc. Jpn*, **77**, 561–568.
Westrip, S. P. (2007). *publCIF*. In preparation.

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supplementary materials

Acta Cryst. (2007). E**63**, o3060 [**doi:10.1107/S1600536807025937**]

(*S*)-(+)-2,2'-Bis(2-hydroxy-3-methoxybenzylideneamino)-1,1'-binaphthyl

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Comment

The nickel derivatives of the Schiff bases that are formed by condensing 2,2'-diamino-1,1-binaphthyl with aldehydes are catalysts for enantioselective Diels-Alder reactions (Suga *et al.*, 2003, 2004). The present crystallographic study follows the study on racemic 2,2'-bis(2-hydroxy-3-ethoxybenzylideneamino)-1,1'-binaphthyl, which exists as a dichloromethane solvate (Che *et al.*, 2002). The title compound is a substitutted 1,1'-binaphthyl that lies on a twofold rotation axis; the fused-rings are twisted by 81.2 (1) ° along the naphthyl–naphthyl bond. The hydroxy group forms an internal hydrogen bond with the imino nitrogen, a feature that is common to Schiff bases derived from a substituted salicyaldehyde such as *o*-vanillin and an amine (Cambridge Structural Database Version 5.28, November 2006).

The structure of the optically active (*S*)-(+)-2,2'-diamino-1,1'-binaphthyl reactant has not been reported although the *R*-enantiomer has already been described (in the $P4_32_12$ space group) (Jones *et al.*, 2003). The space group of the S-enantiomer should be that of the present Schiff base, *i.e.*, $P4_12_12$.

Experimental

(*S*)-(+)-2,2'-Diamino-1,1'-binaphthyl (0.144 g, 0.5 mmol) and *o*-vanillin (0.162 g, 1.05 mmol) was heated in ethanol (10 ml) for several hours. The orange compound that resulted was isolated and recrystallized from ethanol to yield orange prisms of (I) in 70% yield. CH&N elemental analysis: calc. for $C_{36}H_{28}N_2O_4$: C 78.24, H 5.11, N 5.07. Found: C 78.31, H 5.08, N 5.04%.

Refinement

The 2-hydroxy-3-methoxylphenyl part of the molecule is disordered over two positions, the disorder refining to a 0.88:0.22 ratio. The aromatic ring was refined as a rigid hexagon of 1.39 Å sides. Pairs of distances for the unprimed and primed atoms were restrained to within 0.01 Å of each other, and the vibration of the disordered atoms was restrained to be nearly isotropic.

The hydrogen atoms were placed in calculated positions (C—H = 0.93–0.96 Å, O–H 0.82 Å), and refined as riding with $U_{iso}(H) = 1.5U_{eq}$(carrier).

Figures

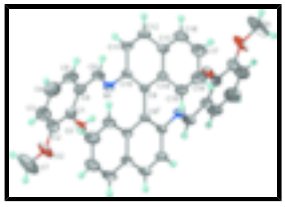


Fig. 1. View of (I) showing 30% displacement ellipsoids. Hydrogen atoms are drawn as spheres of arbitrary radius; the minor disorder component is not shown. Symmetry code (i): $y - 1, 1 + x, 2 - z$.

(*S*)-(+)-2,2'-Bis(2-hydroxy-3-methoxybenzylideneamino)-1,1'-binaphthyl

Crystal data

$C_{36}H_{28}N_2O_4$	$Z = 4$
$M_r = 552.60$	$F_{000} = 1160$
Tetragonal, $P4_12_12$	$D_x = 1.200$ Mg m^{-3}
Hall symbol: P 4abw 2nw	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 11.3285$ (6) Å	Cell parameters from 4468 reflections
$b = 11.3285$ Å	$\theta = 2.5$–21.0º
$c = 23.837$ (1) Å	$\mu = 0.08$ mm^{-1}
$\alpha = 90$º	$T = 295$ (2) K
$\beta = 90$º	Prism, orange
$\gamma = 90$º	0.38 × 0.31 × 0.28 mm
$V = 3059.1$ (2) Å^3	

Data collection

Bruker APEX diffractometer	1190 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	$R_{int} = 0.028$
Monochromator: graphite	$\theta_{max} = 25.0$º
$T = 295$(2) K	$\theta_{min} = 2.0$º
φ and ω scans	$h = -13\rightarrow8$
Absorption correction: none	$k = -13\rightarrow11$
15298 measured reflections	$l = -28\rightarrow28$
1629 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.058$	H-atom parameters constrained
$wR(F^2) = 0.203$	$w = 1/[\sigma^2(F_o^2) + (0.1153P)^2 + 0.6898P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.10$	$(\Delta/\sigma)_{max} = 0.001$
1629 reflections	$\Delta\rho_{max} = 0.19$ e Å^{-3}
240 parameters	$\Delta\rho_{min} = -0.18$ e Å^{-3}
114 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
O1	0.4176 (3)	0.0978 (3)	1.10647 (12)	0.0838 (10)	
H1	0.3736	0.1062	1.0795	0.101*	
N1	0.3657 (3)	0.1225 (3)	1.00195 (13)	0.0697 (10)	
O2'	0.578 (2)	0.061 (2)	1.1879 (8)	0.132 (12)	0.219 (14)
C1'	0.5305 (9)	0.1015 (11)	1.0912 (10)	0.068 (8)	0.219 (14)
C2'	0.6125 (17)	0.0804 (17)	1.1334 (7)	0.086 (8)	0.219 (14)
C3'	0.7324 (14)	0.080 (3)	1.1210 (8)	0.142 (13)	0.219 (14)
H3'	0.7873	0.0663	1.1493	0.170*	0.219 (14)
C4'	0.7703 (9)	0.102 (3)	1.0665 (9)	0.125 (11)	0.219 (14)
H4'	0.8506	0.1015	1.0582	0.150*	0.219 (14)
C5'	0.6883 (15)	0.123 (2)	1.0243 (7)	0.121 (11)	0.219 (14)
H5'	0.7137	0.1367	0.9878	0.146*	0.219 (14)
C6'	0.5684 (13)	0.1226 (13)	1.0366 (8)	0.098 (10)	0.219 (14)
C7'	0.664 (4)	0.038 (3)	1.2268 (11)	0.128 (12)	0.219 (14)
H7A'	0.6278	0.0207	1.2623	0.193*	0.219 (14)
H7B'	0.7132	0.1067	1.2306	0.193*	0.219 (14)
H7C'	0.7104	−0.02725	1.2148	0.193*	0.219 (14)
O2	0.5688 (8)	0.1093 (10)	1.1871 (3)	0.137 (3)	0.781 (14)
C1	0.5282 (4)	0.1316 (6)	1.0922 (3)	0.086 (3)	0.781 (14)
C2	0.6118 (6)	0.1401 (8)	1.1347 (2)	0.105 (3)	0.781 (14)
C3	0.7258 (5)	0.1773 (10)	1.1223 (2)	0.145 (4)	0.781 (14)
H3	0.7818	0.1830	1.1507	0.174*	0.781 (14)
C4	0.7561 (4)	0.2060 (10)	1.0674 (3)	0.145 (4)	0.781 (14)
H4	0.8324	0.2308	1.0592	0.173*	0.781 (14)
C5	0.6724 (5)	0.1974 (8)	1.0250 (2)	0.119 (4)	0.781 (14)
H5	0.6927	0.2166	0.9883	0.143*	0.781 (14)
C6	0.5585 (4)	0.1602 (6)	1.0374 (3)	0.089 (2)	0.781 (14)
C7	0.6429 (16)	0.1174 (15)	1.2321 (4)	0.236 (8)	0.781 (14)
H7A	0.6017	0.0939	1.2655	0.354*	0.781 (14)
H7B	0.6694	0.1975	1.2360	0.354*	0.781 (14)
H7C	0.7097	0.0667	1.2264	0.354*	0.781 (14)
C8	0.4746 (4)	0.1482 (5)	0.99170 (18)	0.0920 (17)	
H8	0.4994	0.1591	0.9549	0.110*	
C9	0.1660 (3)	0.1302 (3)	0.97066 (13)	0.0560 (9)	
C10	0.2827 (4)	0.1112 (4)	0.95811 (14)	0.0630 (11)	
C11	0.3159 (4)	0.0788 (5)	0.90282 (15)	0.0797 (13)	
H11	0.3950	0.0651	0.8948	0.096*	
C12	0.2355 (4)	0.0674 (5)	0.86193 (16)	0.0824 (14)	
H12	0.2598	0.0460	0.8261	0.099*	
C13	0.1139 (4)	0.0876 (4)	0.87250 (16)	0.0743 (12)	
C14	0.0797 (4)	0.1173 (4)	0.92788 (16)	0.0650 (11)	
C15	−0.0424 (4)	0.1352 (6)	0.93804 (19)	0.0926 (16)	
H15	−0.0678	0.1550	0.9739	0.111*	
C16	−0.1225 (6)	0.1239 (8)	0.8962 (2)	0.127 (3)	
H16	−0.2022	0.1361	0.9035	0.153*	

C17	−0.0859 (6)	0.0937 (7)	0.8418 (2)	0.125 (3)
H17	−0.1414	0.0857	0.8133	0.150*
C18	0.0296 (5)	0.0762 (6)	0.83076 (19)	0.1031 (19)
H18	0.0530	0.0562	0.7946	0.124*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.098 (3)	0.093 (2)	0.0602 (16)	−0.013 (2)	−0.0103 (16)	0.0161 (16)
N1	0.063 (2)	0.096 (3)	0.0502 (16)	0.0047 (18)	0.0033 (15)	−0.0002 (18)
O2'	0.165 (19)	0.128 (18)	0.104 (16)	0.008 (13)	−0.074 (13)	0.034 (11)
C1'	0.073 (17)	0.081 (13)	0.051 (13)	0.020 (11)	−0.011 (12)	0.001 (10)
C2'	0.079 (14)	0.093 (17)	0.087 (15)	0.001 (12)	0.008 (12)	−0.011 (12)
C3'	0.13 (2)	0.18 (2)	0.116 (18)	−0.019 (18)	−0.003 (16)	−0.017 (18)
C4'	0.102 (17)	0.18 (2)	0.090 (15)	0.006 (16)	−0.005 (13)	0.011 (16)
C5'	0.074 (15)	0.19 (2)	0.102 (16)	0.039 (15)	−0.007 (13)	−0.001 (16)
C6'	0.072 (16)	0.16 (2)	0.062 (14)	0.010 (14)	0.015 (13)	0.003 (14)
C7'	0.15 (2)	0.114 (18)	0.126 (18)	−0.002 (15)	−0.071 (16)	0.028 (14)
O2	0.156 (6)	0.182 (8)	0.073 (4)	−0.027 (6)	−0.043 (4)	0.046 (4)
C1	0.083 (6)	0.101 (5)	0.073 (6)	0.011 (4)	−0.012 (5)	−0.006 (4)
C2	0.099 (6)	0.127 (8)	0.088 (5)	−0.001 (5)	−0.027 (4)	−0.003 (5)
C3	0.110 (7)	0.228 (13)	0.097 (6)	0.020 (7)	−0.033 (5)	−0.025 (7)
C4	0.066 (4)	0.230 (13)	0.137 (7)	−0.011 (6)	−0.009 (5)	−0.040 (8)
C5	0.072 (5)	0.205 (10)	0.080 (4)	0.005 (6)	0.004 (4)	−0.037 (5)
C6	0.061 (5)	0.129 (6)	0.076 (5)	0.011 (4)	−0.004 (4)	−0.021 (4)
C7	0.219 (14)	0.363 (19)	0.126 (8)	−0.064 (15)	−0.083 (9)	0.075 (11)
C8	0.069 (3)	0.151 (5)	0.056 (2)	−0.001 (3)	0.005 (2)	−0.009 (3)
C9	0.065 (2)	0.059 (2)	0.0437 (18)	0.0001 (17)	0.0039 (17)	−0.0034 (16)
C10	0.067 (2)	0.078 (3)	0.0436 (17)	0.0013 (19)	0.0028 (17)	−0.0034 (18)
C11	0.071 (3)	0.114 (4)	0.053 (2)	0.005 (3)	0.014 (2)	−0.011 (2)
C12	0.087 (3)	0.115 (4)	0.0447 (19)	−0.001 (3)	0.009 (2)	−0.015 (2)
C13	0.082 (3)	0.089 (3)	0.052 (2)	−0.006 (2)	−0.002 (2)	−0.010 (2)
C14	0.071 (3)	0.072 (3)	0.0518 (19)	−0.002 (2)	−0.0041 (19)	−0.0090 (18)
C15	0.076 (3)	0.137 (5)	0.065 (2)	0.007 (3)	−0.006 (2)	−0.023 (3)
C16	0.082 (4)	0.205 (8)	0.095 (4)	0.002 (4)	−0.020 (3)	−0.043 (4)
C17	0.097 (4)	0.196 (8)	0.081 (3)	0.002 (4)	−0.030 (3)	−0.027 (4)
C18	0.103 (4)	0.153 (5)	0.054 (2)	−0.013 (4)	−0.012 (3)	−0.025 (3)

Geometric parameters (Å, °)

O1—C1	1.353 (5)	C4—H4	0.9300
O1—H1	0.8200	C5—C6	1.3900
N1—C8	1.291 (6)	C5—H5	0.9300
N1—C10	1.411 (5)	C6—C8	1.451 (6)
O2'—C7'	1.369 (13)	C7—H7A	0.9600
O2'—C2'	1.378 (11)	C7—H7B	0.9600
C1'—C2'	1.3900	C7—H7C	0.9600
C1'—C6'	1.3900	C8—H8	0.9300
C2'—C3'	1.3900	C9—C10	1.372 (6)

C3'—C4'	1.3900	C9—C14	1.420 (5)
C3'—H3'	0.9300	C9—C9^{i}	1.512 (7)
C4'—C5'	1.3900	C10—C11	1.419 (5)
C4'—H4'	0.9300	C11—C12	1.340 (6)
C5'—C6'	1.3900	C11—H11	0.9300
C5'—H5'	0.9300	C12—C13	1.419 (7)
C7'—H7A'	0.9600	C12—H12	0.9300
C7'—H7B'	0.9600	C13—C18	1.385 (6)
C7'—H7C'	0.9600	C13—C14	1.416 (6)
O2—C7	1.365 (9)	C14—C15	1.419 (7)
O2—C2	1.386 (6)	C15—C16	1.355 (7)
C1—C2	1.3900	C15—H15	0.9300
C1—C6	1.3900	C16—C17	1.403 (8)
C2—C3	1.3900	C16—H16	0.9300
C3—C4	1.3900	C17—C18	1.350 (8)
C3—H3	0.9300	C17—H17	0.9300
C4—C5	1.3900	C18—H18	0.9300
C8—N1—C10	121.1 (4)	C1—C6—C8	121.5 (5)
C7'—O2'—C2'	117.7 (14)	O2—C7—H7A	109.5
C2'—C1'—C6'	120.0	O2—C7—H7B	109.5
O2'—C2'—C1'	121.3 (17)	H7A—C7—H7B	109.5
O2'—C2'—C3'	118.7 (17)	O2—C7—H7C	109.5
C1'—C2'—C3'	120.0	H7A—C7—H7C	109.5
C4'—C3'—C2'	120.0	H7B—C7—H7C	109.5
C4'—C3'—H3'	120.0	N1—C8—C6	120.3 (4)
C2'—C3'—H3'	120.0	N1—C8—H8	119.8
C3'—C4'—C5'	120.0	C6—C8—H8	119.8
C3'—C4'—H4'	120.0	C10—C9—C14	119.4 (3)
C5'—C4'—H4'	120.0	C10—C9—C9^{i}	120.2 (3)
C6'—C5'—C4'	120.0	C14—C9—C9^{i}	120.5 (4)
C6'—C5'—H5'	120.0	C9—C10—N1	117.8 (3)
C4'—C5'—H5'	120.0	C9—C10—C11	119.9 (4)
C5'—C6'—C1'	120.0	N1—C10—C11	122.3 (4)
O2'—C7'—H7A'	109.5	C12—C11—C10	121.4 (4)
O2'—C7'—H7B'	109.5	C12—C11—H11	119.3
H7A'—C7'—H7B'	109.5	C10—C11—H11	119.3
O2'—C7'—H7C'	109.5	C11—C12—C13	121.0 (4)
H7A'—C7'—H7C'	109.5	C11—C12—H12	119.5
H7B'—C7'—H7C'	109.5	C13—C12—H12	119.5
C7—O2—C2	118.4 (8)	C18—C13—C14	120.2 (5)
O1—C1—C2	117.9 (5)	C18—C13—C12	121.8 (4)
O1—C1—C6	122.1 (5)	C14—C13—C12	118.0 (4)
C2—C1—C6	120.0	C13—C14—C15	117.4 (4)
O2—C2—C3	126.5 (6)	C13—C14—C9	120.4 (4)
O2—C2—C1	113.5 (6)	C15—C14—C9	122.3 (4)
C3—C2—C1	120.0	C16—C15—C14	120.9 (5)
C4—C3—C2	120.0	C16—C15—H15	119.5
C4—C3—H3	120.0	C14—C15—H15	119.5

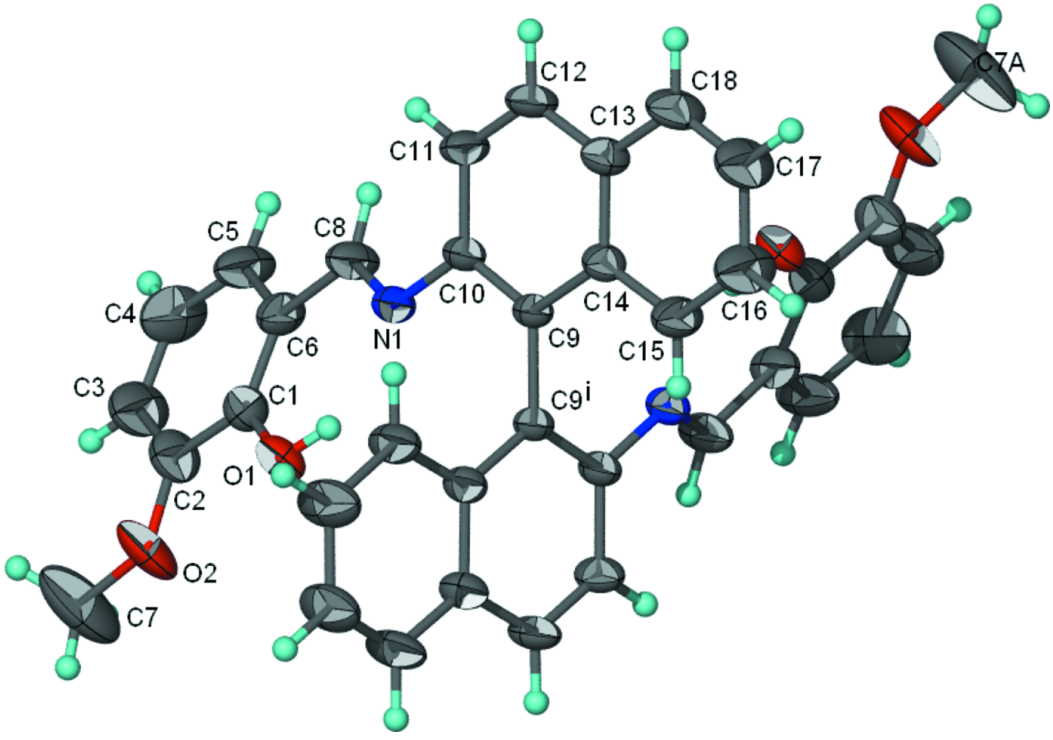
C2—C3—H3	120.0	C15—C16—C17	120.3 (6)
C3—C4—C5	120.0	C15—C16—H16	119.8
C3—C4—H4	120.0	C17—C16—H16	119.8
C5—C4—H4	120.0	C18—C17—C16	120.2 (5)
C6—C5—C4	120.0	C18—C17—H17	119.9
C6—C5—H5	120.0	C16—C17—H17	119.9
C4—C5—H5	120.0	C17—C18—C13	120.9 (5)
C5—C6—C1	120.0	C17—C18—H18	119.5
C5—C6—C8	118.5 (5)	C13—C18—H18	119.5
C7'—O2'—C2'—C1'	178.9 (8)	C1—C6—C8—N1	7.5 (7)
C7'—O2'—C2'—C3'	−1.8 (14)	C14—C9—C10—N1	−178.7 (4)
C6'—C1'—C2'—O2'	179.3 (7)	C9^{i}—C9—C10—N1	2.0 (6)
C6'—C1'—C2'—C3'	0.0	C14—C9—C10—C11	−0.1 (6)
O2'—C2'—C3'—C4'	−179.3 (6)	C9^{i}—C9—C10—C11	−179.3 (4)
C1'—C2'—C3'—C4'	0.0	C8—N1—C10—C9	−154.8 (4)
C2'—C3'—C4'—C5'	0.0	C8—N1—C10—C11	26.6 (7)
C3'—C4'—C5'—C6'	0.0	C9—C10—C11—C12	0.8 (7)
C4'—C5'—C6'—C1'	0.0	N1—C10—C11—C12	179.4 (5)
C2'—C1'—C6'—C5'	0.0	C10—C11—C12—C13	0.1 (8)
C7—O2—C2—C3	1.4 (11)	C11—C12—C13—C18	−180.0 (5)
C7—O2—C2—C1	−178.3 (7)	C11—C12—C13—C14	−1.5 (8)
O1—C1—C2—O2	1.3 (6)	C18—C13—C14—C15	−0.4 (7)
C6—C1—C2—O2	179.7 (5)	C12—C13—C14—C15	−178.9 (5)
O1—C1—C2—C3	−178.4 (4)	C18—C13—C14—C9	−179.4 (5)
C6—C1—C2—C3	0.0	C12—C13—C14—C9	2.1 (7)
O2—C2—C3—C4	−179.7 (5)	C10—C9—C14—C13	−1.4 (6)
C1—C2—C3—C4	0.0	C9^{i}—C9—C14—C13	177.9 (4)
C2—C3—C4—C5	0.0	C10—C9—C14—C15	179.8 (5)
C3—C4—C5—C6	0.0	C9^{i}—C9—C14—C15	−1.0 (6)
C4—C5—C6—C1	0.0	C13—C14—C15—C16	0.1 (9)
C4—C5—C6—C8	−177.8 (4)	C9—C14—C15—C16	179.0 (6)
O1—C1—C6—C5	178.4 (5)	C14—C15—C16—C17	0.2 (11)
C2—C1—C6—C5	0.0	C15—C16—C17—C18	−0.3 (13)
O1—C1—C6—C8	−3.9 (5)	C16—C17—C18—C13	0.0 (12)
C2—C1—C6—C8	177.7 (4)	C14—C13—C18—C17	0.4 (10)
C10—N1—C8—C6	179.6 (4)	C12—C13—C18—C17	178.8 (6)
C5—C6—C8—N1	−174.8 (4)		

Symmetry codes: (i) *y*, *x*, −*z*+2.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1	0.82	1.86	2.575 (4)	145

Fig. 1


C12
C18
C7A
C13
C11
C17
C5
C8
C10
C14
C16
C4
N1
C6
C9
C15
C3
C1
C9i
O1
C2
O2
C7