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4-(2-Hydroxyphenyliminomethylene)phenol

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.043
wR factor = 0.087
Data-to-parameter ratio = 15.9

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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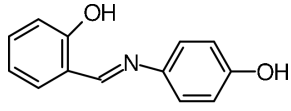
The asymmetric unit of the title compound, $C_{13}H_{11}NO_2$, consists of two crystallographically independent molecules which are essentially planar and are approximately orthogonal to each other. These two molecules are linked by an O—H···O hydrogen bond and display two intramolecular O—H···N hydrogen bonds.

Comment

Schiff bases have been extensively used as ligands in the field of coordination chemistry (Calligaris *et al.*, 1972; Garnovski *et al.*, 1993). Schiff base compounds can be classified by their photochromic and thermochromic characteristics (Cohen *et al.*, 1964; Moustakali *et al.*, 1978; Hadjoudis *et al.*, 1987). Based on studies of some thermochromic and photochromic Schiff base compounds, it has been proposed that molecules exhibiting monochromism are planar, while those exhibiting photochromism are non-planar (Moustakali *et al.*, 1978). Our structural investigations of Schiff bases (Kazak *et al.*, 2000; Ersanlı *et al.*, 2003; Odabaşoğlu *et al.*, 2003) have led us to examine the title compound, (I).



(I)

The asymmetric unit of (I) consists of two crystallographically independent, but nearly identical, molecules (*A* and *B*) linked by an O—H···O hydrogen bond (Fig. 1 and

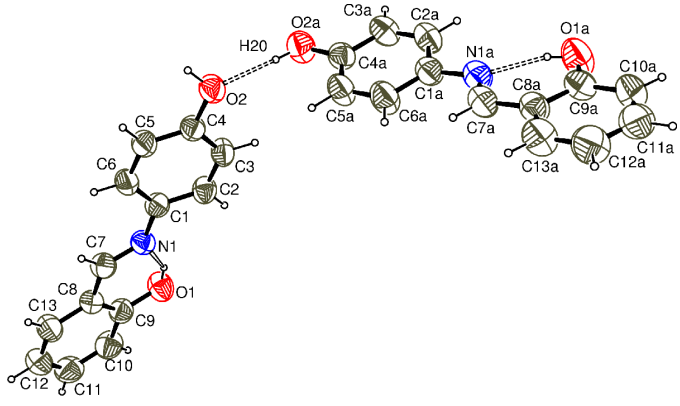


Figure 1
ORTEP view (Burnett & Johnson, 1996; Farrugia, 1997) of the asymmetric unit of (I), showing the atom-labelling scheme. Ellipsoids are drawn at the 50% probability level. H atoms are represented as spheres of arbitrary radius. The open dashed lines indicate hydrogen bonds.

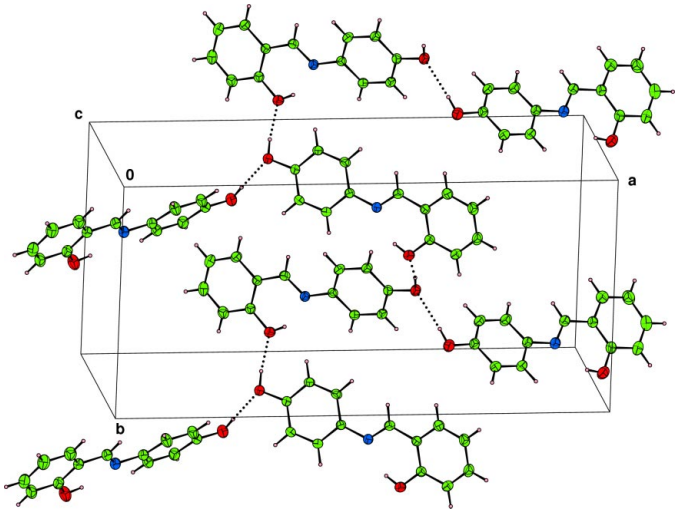


Figure 2
CAMERON (Watkin *et al.*, 1996) packing diagram for (I), showing the O—H···O hydrogen-bonding intercations as dashed lines. Ellipsoids are drawn at the 20% probability level. The H atoms are represented as spheres of arbitrary radius.

Table 2). The two molecules make a dihedral angle of 73.07 (4)°. They are both roughly planar, the largest deviation being 0.225 (2) Å at C2 for molecule *A* and 0.160 (2) Å at atom C6*A* for molecule *B*. However, the benzene ring C1–C6 (C1*A*–C6*A*) is slightly twisted with respect to the C1—N1═C7—C8 (C1*A*—N1*A*═C7*A*—C8*A*) moiety, as indicated by the value of the dihedral angle between these planes 12.3 (1)° [9.7 (3)°]. The two other benzene rings, C8–C13 and C8*A*–C13*A*, are less twisted with respect to the imino groups, the dihedral angles being 3.5 (1) and 1.1 (3)°, respectively.

The C—O (hydroxyl) bonds [1.350 (2) and 1.355 (3) Å in molecules *A* and *B*, respectively] indicate single-bond character, whereas the N—C bonds [1.286 (2) and 1.278 (3) Å in molecules *A* and *B*, respectively] show double-bond character. These bond lengths are consistent with typical values reported in related compounds (Kevran *et al.*, 1996; Elerman & Elmalı, 1998). The enol–imine tautomeric form is favoured over the keto–amine form.

There are strong intramolecular hydrogen bonds O1—H1···N1 and O1*A*—H1*A*···N1*A* (Table 2). The sum of the van der Walls radii of O and N (3.07 Å; Bondi, 1964) is significantly longer than the O···N hydrogen-bond length; similar results were observed in *N*-(3,5-dichorophenyl)-naphthaldimine [2.570 (3) Å; Elmali *et al.*, 1998] and in 5-chloro-2-[(2-hydroxybenzylidene)aminomethyl]phenol [2.599 (3) Å; Kevran *et al.*, 1996]. The packing of the molecules within the crystals is governed by O—H···O hydrogen-bonding interactions (Table 2 and Fig. 2)

Experimental

The title compound, (I), was prepared as described by Ersanlı *et al.* (2003), using salicylaldehyde and 4-hydroxyaniline as starting materials. The product was recrystallized from ethanol and well shaped crystals of (I) were obtained by slow evaporation of an ethanol solution (yield 85%; m.p. 405–407 K).

Crystal data

$C_{13}H_{11}NO_2$
M_r = 213.23
Monoclinic, $P2_1/c$
a = 22.041 (5) Å
b = 10.820 (5) Å
c = 8.924 (5) Å
β = 91.550 (5)°
V = 2127.4 (16) Å^3
Z = 8
D_x = 1.331 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 7947 reflections
θ = 1.9–27.2°
μ = 0.09 mm^{-1}
T = 293 (2) K
Prism, brown
0.38 × 0.26 × 0.12 mm

Data collection

Stoe IPDS-II diffractometer
ω scans
Absorption correction: by integration (*X-RED*32; Stoe & Cie, 2002)
T_{min} = 0.973, T_{max} = 0.990
28099 measured reflections
4693 independent reflections
1919 reflections with $I > 2\sigma(I)$
R_{int} = 0.129
θ_{max} = 27.2°
$h = -25 \rightarrow 28$
$k = -13 \rightarrow 13$
$l = -11 \rightarrow 11$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.087
S = 0.73
4693 reflections
295 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0434P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C1—N1	1.423 (2)	C7—N1	1.285 (2)
C1*A*—N1*A*	1.418 (2)	C7*A*—N1*A*	1.278 (2)
C4—O2	1.3741 (19)	C9—O1	1.350 (2)
C4*A*—O2*A*	1.375 (2)	C9*A*—O1*A*	1.355 (2)
C2—C1—N1	116.91 (15)	N1—C7—C8	121.68 (16)
C6—C1—N1	124.66 (15)	N1*A*—C7*A*—C8*A*	122.08 (18)
C2*A*—C1*A*—N1*A*	116.90 (17)	O1—C9—C10	119.97 (16)
C6*A*—C1*A*—N1*A*	125.13 (19)	O1—C9—C8	120.53 (15)
C3—C4—O2	118.30 (15)	O1*A*—C9*A*—C10*A*	118.5 (2)
O2—C4—C5	122.13 (15)	O1*A*—C9*A*—C8*A*	121.35 (19)
C5*A*—C4*A*—O2*A*	122.93 (17)	C7—N1—C1	124.07 (14)
C3*A*—C4A—O2*A*	117.69 (18)	C7*A*—N1*A*—C1*A*	122.12 (17)
C1—N1—C7—C8	179.91 (15)	N1*A*—C7*A*—C8*A*—C9*A*	−0.8 (3)
N1—C7—C8—C9	−3.4 (3)	C7—N1—C1—C6	−12.5 (3)
N1—C7—C8—C13	176.67 (17)	C7—N1—C1—C2	167.90 (17)
C1*A*—N1*A*—C7*A*—C8*A*	179.57 (17)	C7*A*—N1*A*—C1*A*—C6*A*	−9.9 (3)
N1*A*—C7*A*—C8*A*—C13*A*	179.57 (18)	C7*A*—N1*A*—C1*A*—C2*A*	170.83 (17)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1	0.82	1.81	2.5465 (19)	149
O1*A*—H1*A*···N1*A*	0.82	1.86	2.591 (2)	147
O2—H21···O1^{i}	0.878 (14)	1.889 (14)	2.757 (2)	169.9 (18)
O2*A*—H20···O2	0.847 (15)	2.006 (15)	2.852 (2)	177 (2)

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

All H atoms, except for those of the two terminal hydroxy groups (O2 and O2*A*), were placed in calculated positions (O—H = 0.82 Å and C—H = 0.93 Å), with U_{iso} values constrained to be $1.5U_{eq}$ of the carrier atom for the hydroxyl-group H atom and $1.2U_{eq}$ for the remaining H atoms. The coordinates of the H atoms of the two

terminal hydroxy groups were refined with the O—H distances restrained to 0.82 (2) Å and isotropic displacement parameters constrained to be $1.2U_{eq}$(O).

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED*32 (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*III (Burnett & Johnson, 1996), *ORTEP*-3 *for Window*s (Farrugia, 1997) and *CAMERON* (Watkin *et al.*, 1996); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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4-(2-Hydroxyphenyliminomethylene)phenol

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Crystal data

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$M_r = 213.23$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 22.041$ (5) Å
$b = 10.820$ (5) Å
$c = 8.924$ (5) Å
$\beta = 91.550$ (5)°
$V = 2127.4$ (16) Å^3
$Z = 8$
$F(000) = 896$
$D_x = 1.331$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71069$ Å
Cell parameters from 7947 reflections
$\theta = 1.9$–27.2°
$\mu = 0.09$ mm^{-1}
$T = 293$ K
Prism, brown
0.38 × 0.26 × 0.12 mm

Data collection

Stoe IPDS-II diffractometer
Radiation source: fine-focus sealed tube
Plane graphite monochromator
Detector resolution: 6.67 pixels mm^{-1}
ω scans
Absorption correction: integration (X-RED32; Stoe & Cie, 2002)
$T_{min} = 0.973$, $T_{max} = 0.990$
28099 measured reflections
4693 independent reflections
1919 reflections with $I > 2\sigma(I)$
$R_{int} = 0.13$
$\theta_{max} = 27.2°$, $\theta_{min} = 1.9°$
$h = -25 \rightarrow 28$
$k = -13 \rightarrow 13$
$l = -11 \rightarrow 11$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.043$
$wR(F^2) = 0.087$
$S = 0.73$
4693 reflections
295 parameters
2 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0434P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.33$ e Å^{-3}
$\Delta\rho_{min} = -0.24$ e Å^{-3}

Special details

Experimental. The crystal used for data collection was very thin and the quality of the data were poor as shown by the high value of R_{int} equal to 0.13, the least squares goodness of fit parameter of 0.726 and the very low ratio Observed/Unique reflections of 41%.

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.50378 (7)	0.28374 (15)	0.12481 (19)	0.0475 (4)
C1A	0.12039 (9)	0.11268 (17)	0.3145 (2)	0.0583 (5)
C2	0.46044 (8)	0.19610 (15)	0.1548 (2)	0.0528 (5)
H2	0.4644	0.1169	0.1157	0.063*
C2A	0.13952 (9)	0.04671 (17)	0.4394 (2)	0.0651 (5)
H2A	0.1131	−0.0090	0.4829	0.078*
C3	0.41133 (8)	0.22326 (16)	0.2417 (2)	0.0547 (5)
H3	0.3826	0.1628	0.2609	0.066*
C3A	0.19705 (9)	0.06197 (17)	0.5006 (2)	0.0667 (5)
H3A	0.2091	0.0168	0.5849	0.080*
C4	0.40507 (8)	0.34000 (15)	0.29974 (19)	0.0492 (4)
C4A	0.23656 (8)	0.14364 (16)	0.4375 (2)	0.0567 (5)
C5	0.44752 (8)	0.42928 (15)	0.2688 (2)	0.0561 (5)
H5	0.4430	0.5088	0.3063	0.067*
C5A	0.21866 (9)	0.20758 (18)	0.3118 (2)	0.0688 (6)
H5A	0.2456	0.2618	0.2674	0.083*
C6	0.49673 (8)	0.40140 (15)	0.18229 (19)	0.0557 (5)
H6	0.5253	0.4621	0.1626	0.067*
C6A	0.16131 (9)	0.19264 (19)	0.2503 (2)	0.0746 (6)
H6A	0.1498	0.2367	0.1647	0.090*
C7	0.59142 (8)	0.31990 (16)	−0.02141 (19)	0.0524 (5)
H7	0.5871	0.4044	−0.0061	0.063*
C7A	0.03509 (9)	0.15875 (18)	0.1587 (2)	0.0647 (5)
H7A	0.0571	0.2236	0.1185	0.078*
C8	0.64057 (7)	0.27600 (15)	−0.10930 (18)	0.0481 (4)
C8A	−0.02604 (9)	0.13692 (17)	0.1037 (2)	0.0607 (5)
C9	0.65067 (8)	0.14915 (16)	−0.1285 (2)	0.0529 (4)
C9A	−0.06095 (9)	0.04030 (19)	0.1580 (2)	0.0655 (5)
C10	0.69856 (9)	0.10988 (18)	−0.2150 (2)	0.0667 (5)
H10	0.7056	0.0258	−0.2277	0.080*
C10A	−0.11941 (10)	0.0208 (2)	0.1010 (3)	0.0799 (6)
H10A	−0.1426	−0.0442	0.1368	0.096*
C11	0.73536 (9)	0.1944 (2)	−0.2814 (2)	0.0723 (6)
H11	0.7670	0.1673	−0.3399	0.087*
C11A	−0.14290 (10)	0.0974 (2)	−0.0080 (3)	0.0847 (7)
H11A	−0.1822	0.0843	−0.0453	0.102*

C12	0.72588 (9)	0.3193 (2)	−0.2625 (2)	0.0693 (6)
H12	0.7512	0.3760	−0.3078	0.083*
C12A	−0.10933 (11)	0.1934 (2)	−0.0630 (3)	0.0892 (7)
H12A	−0.1256	0.2447	−0.1374	0.107*
C13	0.67934 (8)	0.36007 (17)	−0.1772 (2)	0.0610 (5)
H13	0.6734	0.4445	−0.1642	0.073*
C13A	−0.05172 (10)	0.2124 (2)	−0.0070 (3)	0.0818 (6)
H13A	−0.0291	0.2777	−0.0440	0.098*
N1	0.55324 (6)	0.24542 (13)	0.03668 (15)	0.0494 (4)
N1A	0.06008 (7)	0.09177 (15)	0.26097 (18)	0.0630 (4)
O1	0.61451 (6)	0.06526 (10)	−0.06328 (15)	0.0653 (4)
H1	0.5885	0.1012	−0.0158	0.098*
O1A	−0.03884 (6)	−0.03746 (14)	0.26524 (17)	0.0901 (5)
H1A	−0.0041	−0.0169	0.2895	0.135*
O2	0.35594 (6)	0.36379 (11)	0.38679 (14)	0.0605 (4)
H21	0.3617 (8)	0.4326 (14)	0.437 (2)	0.073*
O2A	0.29319 (6)	0.15613 (13)	0.50410 (16)	0.0720 (4)
H20	0.3105 (9)	0.2187 (16)	0.467 (2)	0.086*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0477 (10)	0.0463 (9)	0.0484 (10)	0.0010 (8)	0.0009 (9)	−0.0012 (8)
C1A	0.0557 (12)	0.0560 (11)	0.0637 (13)	−0.0019 (9)	0.0107 (10)	−0.0009 (10)
C2	0.0526 (11)	0.0431 (9)	0.0627 (12)	−0.0013 (8)	0.0032 (10)	−0.0040 (8)
C2A	0.0613 (13)	0.0606 (12)	0.0742 (14)	−0.0069 (10)	0.0146 (11)	0.0083 (10)
C3	0.0506 (11)	0.0472 (10)	0.0667 (12)	−0.0079 (8)	0.0051 (10)	−0.0029 (9)
C3A	0.0643 (14)	0.0667 (12)	0.0695 (14)	0.0010 (11)	0.0106 (11)	0.0136 (10)
C4	0.0446 (10)	0.0511 (10)	0.0523 (11)	0.0000 (8)	0.0046 (9)	−0.0032 (8)
C4A	0.0532 (12)	0.0558 (11)	0.0616 (13)	0.0005 (9)	0.0108 (10)	−0.0053 (10)
C5	0.0615 (12)	0.0454 (10)	0.0622 (12)	−0.0060 (9)	0.0137 (10)	−0.0086 (8)
C5A	0.0624 (14)	0.0701 (13)	0.0744 (15)	−0.0130 (10)	0.0090 (12)	0.0145 (11)
C6	0.0613 (12)	0.0481 (10)	0.0584 (12)	−0.0114 (9)	0.0137 (10)	−0.0029 (9)
C6A	0.0657 (14)	0.0841 (14)	0.0741 (15)	−0.0139 (11)	0.0026 (12)	0.0227 (11)
C7	0.0567 (11)	0.0469 (10)	0.0536 (11)	0.0024 (9)	0.0028 (10)	0.0005 (8)
C7A	0.0600 (13)	0.0607 (12)	0.0739 (15)	−0.0031 (10)	0.0141 (11)	0.0022 (11)
C8	0.0485 (10)	0.0491 (10)	0.0467 (10)	−0.0004 (8)	0.0026 (9)	−0.0005 (8)
C8A	0.0556 (12)	0.0605 (12)	0.0666 (13)	0.0009 (10)	0.0111 (10)	−0.0014 (10)
C9	0.0504 (11)	0.0547 (11)	0.0537 (11)	−0.0011 (9)	0.0004 (9)	−0.0036 (9)
C9A	0.0586 (13)	0.0723 (13)	0.0663 (14)	0.0028 (11)	0.0126 (11)	0.0003 (11)
C10	0.0618 (13)	0.0644 (12)	0.0742 (14)	0.0068 (10)	0.0078 (11)	−0.0161 (11)
C10A	0.0604 (15)	0.0943 (17)	0.0857 (17)	−0.0116 (12)	0.0149 (13)	−0.0037 (14)
C11	0.0560 (12)	0.0955 (17)	0.0659 (13)	0.0013 (12)	0.0122 (11)	−0.0184 (12)
C11A	0.0620 (14)	0.1117 (19)	0.0805 (17)	0.0047 (14)	0.0042 (13)	−0.0104 (15)
C12	0.0604 (13)	0.0836 (15)	0.0645 (14)	−0.0119 (11)	0.0137 (11)	−0.0005 (11)
C12A	0.0725 (16)	0.1065 (19)	0.0882 (18)	0.0104 (14)	−0.0023 (14)	0.0107 (14)
C13	0.0610 (12)	0.0569 (11)	0.0657 (12)	−0.0048 (10)	0.0107 (10)	0.0023 (10)
C13A	0.0735 (15)	0.0833 (15)	0.0889 (17)	0.0010 (12)	0.0048 (13)	0.0126 (13)

N1	0.0477 (8)	0.0508 (8)	0.0500 (9)	−0.0007 (7)	0.0052 (7)	−0.0006 (7)
N1A	0.0564 (11)	0.0655 (10)	0.0676 (11)	−0.0022 (8)	0.0105 (9)	0.0010 (8)
O1	0.0651 (8)	0.0481 (7)	0.0836 (9)	0.0002 (6)	0.0146 (7)	−0.0009 (6)
O1A	0.0719 (10)	0.0976 (11)	0.1009 (12)	−0.0151 (8)	0.0059 (9)	0.0304 (9)
O2	0.0547 (8)	0.0567 (8)	0.0708 (9)	−0.0050 (6)	0.0148 (7)	−0.0092 (6)
O2A	0.0599 (9)	0.0775 (10)	0.0787 (10)	−0.0063 (7)	0.0032 (8)	0.0054 (8)

Geometric parameters (Å, º)

C1—C2	1.377 (2)	C7A—C8A	1.441 (3)
C1—C6	1.383 (2)	C7A—H7A	0.9300
C1—N1	1.423 (2)	C8—C13	1.397 (2)
C1A—C2A	1.380 (3)	C8—C9	1.402 (2)
C1A—C6A	1.385 (3)	C8A—C13A	1.390 (3)
C1A—N1A	1.418 (2)	C8A—C9A	1.393 (3)
C2—C3	1.380 (2)	C9—O1	1.350 (2)
C2—H2	0.9300	C9—C10	1.391 (2)
C2A—C3A	1.377 (3)	C9A—O1A	1.355 (2)
C2A—H2A	0.9300	C9A—C10A	1.389 (3)
C3—C4	1.374 (2)	C10—C11	1.368 (3)
C3—H3	0.9300	C10—H10	0.9300
C3A—C4A	1.372 (2)	C10A—C11A	1.369 (3)
C3A—H3A	0.9300	C10A—H10A	0.9300
C4—O2	1.3741 (19)	C11—C12	1.379 (3)
C4—C5	1.378 (2)	C11—H11	0.9300
C4A—C5A	1.367 (3)	C11A—C12A	1.373 (3)
C4A—O2A	1.375 (2)	C11A—H11A	0.9300
C5—C6	1.381 (2)	C12—C13	1.367 (2)
C5—H5	0.9300	C12—H12	0.9300
C5A—C6A	1.374 (3)	C12A—C13A	1.367 (3)
C5A—H5A	0.9300	C12A—H12A	0.9300
C6—H6	0.9300	C13—H13	0.9300
C6A—H6A	0.9300	C13A—H13A	0.9300
C7—N1	1.285 (2)	O1—H1	0.8200
C7—C8	1.435 (2)	O1A—H1A	0.8200
C7—H7	0.9300	O2—H21	0.878 (14)
C7A—N1A	1.278 (2)	O2A—H20	0.847 (15)
C2—C1—C6	118.43 (15)	C13—C8—C9	118.91 (16)
C2—C1—N1	116.91 (15)	C13—C8—C7	120.05 (16)
C6—C1—N1	124.66 (15)	C9—C8—C7	121.04 (15)
C2A—C1A—C6A	117.97 (19)	C13A—C8A—C9A	118.0 (2)
C2A—C1A—N1A	116.90 (17)	C13A—C8A—C7A	120.32 (19)
C6A—C1A—N1A	125.13 (19)	C9A—C8A—C7A	121.65 (19)
C1—C2—C3	121.42 (15)	O1—C9—C10	119.97 (16)
C1—C2—H2	119.3	O1—C9—C8	120.53 (15)
C3—C2—H2	119.3	C10—C9—C8	119.50 (16)
C3A—C2A—C1A	121.10 (18)	O1A—C9A—C10A	118.5 (2)

C3A—C2A—H2A	119.5	O1A—C9A—C8A	121.35 (19)
C1A—C2A—H2A	119.5	C10A—C9A—C8A	120.2 (2)
C4—C3—C2	119.73 (15)	C11—C10—C9	120.28 (18)
C4—C3—H3	120.1	C11—C10—H10	119.9
C2—C3—H3	120.1	C9—C10—H10	119.9
C4A—C3A—C2A	120.14 (19)	C11A—C10A—C9A	119.8 (2)
C4A—C3A—H3A	119.9	C11A—C10A—H10A	120.1
C2A—C3A—H3A	119.9	C9A—C10A—H10A	120.1
C3—C4—O2	118.30 (15)	C10—C11—C12	120.56 (19)
C3—C4—C5	119.57 (16)	C10—C11—H11	119.7
O2—C4—C5	122.13 (15)	C12—C11—H11	119.7
C5A—C4A—C3A	119.37 (19)	C10A—C11A—C12A	121.0 (2)
C5A—C4A—O2A	122.93 (17)	C10A—C11A—H11A	119.5
C3A—C4A—O2A	117.69 (18)	C12A—C11A—H11A	119.5
C4—C5—C6	120.43 (16)	C13—C12—C11	120.20 (19)
C4—C5—H5	119.8	C13—C12—H12	119.9
C6—C5—H5	119.8	C11—C12—H12	119.9
C4A—C5A—C6A	120.66 (18)	C13A—C12A—C11A	119.1 (2)
C4A—C5A—H5A	119.7	C13A—C12A—H12A	120.4
C6A—C5A—H5A	119.7	C11A—C12A—H12A	120.4
C5—C6—C1	120.41 (16)	C12—C13—C8	120.55 (18)
C5—C6—H6	119.8	C12—C13—H13	119.7
C1—C6—H6	119.8	C8—C13—H13	119.7
C5A—C6A—C1A	120.7 (2)	C12A—C13A—C8A	121.8 (2)
C5A—C6A—H6A	119.6	C12A—C13A—H13A	119.1
C1A—C6A—H6A	119.6	C8A—C13A—H13A	119.1
N1—C7—C8	121.68 (16)	C7—N1—C1	124.07 (14)
N1—C7—H7	119.2	C7A—N1A—C1A	122.12 (17)
C8—C7—H7	119.2	C9—O1—H1	109.5
N1A—C7A—C8A	122.08 (18)	C9A—O1A—H1A	109.5
N1A—C7A—H7A	119.0	C4—O2—H21	110.1 (12)
C8A—C7A—H7A	119.0	C4A—O2A—H20	108.9 (15)
C1—N1—C7—C8	179.91 (15)	N1A—C7A—C8A—C9A	−0.8 (3)
N1—C7—C8—C9	−3.4 (3)	C7—N1—C1—C6	−12.5 (3)
N1—C7—C8—C13	176.67 (17)	C7—N1—C1—C2	167.90 (17)
C1A—N1A—C7A—C8A	179.57 (17)	C7A—N1A—C1A—C6A	−9.9 (3)
N1A—C7A—C8A—C13A	179.57 (18)	C7A—N1A—C1A—C2A	170.83 (17)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1	0.82	1.81	2.5465 (19)	149
O1*A*—H1*A*···N1*A*	0.82	1.86	2.591 (2)	147
O2—H21···O1^{i}	0.88 (1)	1.89 (1)	2.757 (2)	170 (2)
O2*A*—H20···O2	0.85 (2)	2.01 (2)	2.852 (2)	177 (2)

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