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A chiral photochromic Schiff base: (*R*)-4-methoxy-2-[(1-phenylethyl)imino-methyl]phenol

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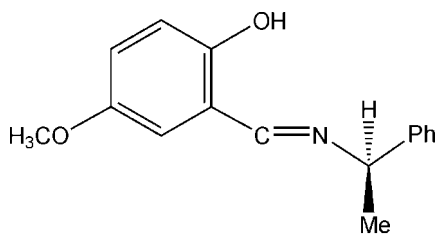
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 Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.042; wR factor = 0.088; data-to-parameter ratio = 7.0.

The title chiral photochromic Schiff base compound, $\text{C}_{16}\text{H}_{17}\text{NO}_2$, was synthesized from (*R*)-1-phenylethylamine and 5-methoxysalicylaldehyde. The molecule of the title compound exists in the phenol-imine tautomeric form. The dihedral angle between the two aromatic rings is $62.61(11)^\circ$. An intramolecular $\text{O}-\text{H}\cdots\text{N}$ hydrogen bond with an $\text{O}\cdots\text{N}$ distance of $2.589(2)$ Å is observed. The crystal packing is stabilized by $\text{C}-\text{H}\cdots\pi$ interactions involving the aromatic ring.

Related literature

For chiral metal complexes and their hybrid materials, see: Akitsu (2007); Akitsu & Einaga (2004, 2005*a,b*, 2006*a*); Akitsu *et al.* (2009); Yamada (1999). For structural comparison of the 1-phenylethylamine moiety, see: Antonov *et al.* (1995); Liu *et al.* (1997). For related Schiff base ligands and their functions, see: Akitsu *et al.* (2004); Akitsu & Einaga (2006*b*); Hadjoudis *et al.* (1987, 2004); Santoni & Rehder (2004); Sliwa *et al.* (2005).



Experimental

Crystal data

$\text{C}_{16}\text{H}_{17}\text{NO}_2$
 $M_r = 255.31$
 Monoclinic, $P2_1$
 $a = 8.270(4)$ Å
 $b = 5.886(3)$ Å

$c = 13.920(7)$ Å
 $\beta = 93.254(7)^\circ$
 $V = 676.4(6)$ Å³
 $Z = 2$
 Mo $K\alpha$ radiation

$\mu = 0.08$ mm⁻¹
 $T = 100$ K

$0.21 \times 0.19 \times 0.07$ mm

Data collection

Bruker SMART CCD
 area-detector diffractometer
 Absorption correction: multi-scan
 (SADABS; Bruker, 1998)
 $T_{\min} = 0.983$, $T_{\max} = 0.994$

3805 measured reflections
 1677 independent reflections
 1454 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.074$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.042$
 $wR(F^2) = 0.088$
 $S = 0.99$
 1677 reflections
 240 parameters

1 restraint
 All H-atom parameters refined
 $\Delta\rho_{\max} = 0.31$ e Å⁻³
 $\Delta\rho_{\min} = -0.18$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{O1}-\text{H1}\cdots\text{N1}$	0.97 (3)	1.72 (5)	2.589 (2)	151 (3)
$\text{C12}-\text{H12}\cdots\text{Cg1}^{\text{i}}$	1.03 (4)	2.72 (3)	3.536 (3)	137 (3)
$\text{C16}-\text{H16C}\cdots\text{Cg1}^{\text{ii}}$	0.98 (4)	2.71 (3)	3.563 (3)	149 (3)

Symmetry codes: (i) $-x + 1, y + \frac{1}{2}, -z + 1$; (ii) $-x, y - \frac{1}{2}, -z$. Cg 1 is the centroid of the C10–C15 ring.

Data collection: SMART (Bruker, 1998); cell refinement: SAINT (Bruker, 1998); 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: SHELXL97.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2897).

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supporting information

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A chiral photochromic Schiff base: (*R*)-4-methoxy-2-[(1-phenylethyl)imino-methyl]phenol

Yukie Miura, Yoshikazu Aritake and Takashiro Akitsu

S1. Comment

Because of structural flexibility and their application for switching materials and so on, Schiff base compounds are one of the most extensively used ligands in the field of coordination chemistry (Yamada, 1999). Especially, aiming at multifunctional chiral materials, we have investigated Schiff base Cu^{II}, Ni^{II}, or Zn^{II} complexes in view of thermally induced structural phase transition in the solid state (Akitsu & Einaga, 2004), structural change by occlusion of solvents (Akitsu & Einaga, 2005*a*), chiral conformational change in a solution induced by a photochromic solute (Akitsu & Einaga, 2005*b*, 2006*a*; Akitsu, 2007), and novel induced CD to achiral metallodendrimers (Akitsu *et al.*, 2009). On the other hand, free Schiff base ligands (Akitsu *et al.*, 2004, Akitsu & Einaga, 2006*b*) have been also studied as multifunctional components, for example photochromic and thermochromic or fluorescence materials (Hadjoudis *et al.*, 2004) and nonlinear optical materials (Sliwa *et al.*, 2005) and so on. In order to clarify the role of electron-donating methoxy group, as free ligands for tautomerism and photochromism (Hadjoudis *et al.*, 1987), crystal structure of the title compound, (I), has been determined.

Crystal structure of (I) is similar to those of the analogous derivatives (Santoni & Rehder, 2004; Akitsu & Einaga, 2006*b*). Molecule of (I) (Fig. 1) adopts an E configuration with respect to the imine C=N double bond with a C6—C7—N1—C8 torsion angle of -179.40 (18)°. Thus, the π -conjugate system around the imine group is essentially planar. The C1—O1 bond distance of 1.361 (3) Å suggests that it is in the phenol-imine tautomer. The contraction of the C7=N1 bond [1.283 (3) Å] is also in agreement with the phenol-imine tautomer. As for the methoxy group, the O2—C4 and O2—C16 bond distances are 1.374 (3) and 1.422 (3) Å, respectively, and the C4—O2—C16 bond angle is 116.9 (2)°. Beside them, geometric parameters reported here agree with corresponding values reported for analogous Schiff base compounds containing the 1-phenylethylamine group (Antonov *et al.*, 1995; Liu *et al.*, 1997). The planarity of (I) is stabilized by an intramolecular O—H \cdots N hydrogen bond (Table 1). However, there is no intermolecular hydrogen bonds associated with the methoxy group. The crystal packing is stabilized by C—H \cdots π interactions involving the C10-C15 ring.

S2. Experimental

Treatment of equimolar *R*-1-phenylethylamine and 5-methoxysalicylaldehyde in methanol at 298 K overnight gave rise to a yellow-green compound (I). Prismatic crystals of (I) were grown from the resulting solution over a period of several days (yield 39.0%). Analysis found: C 73.98, H 6.49, N 5.37%; calculated for C₁₆H₁₇NO₂: C 75.27, H 6.71, N, 5.49%. (precipitates containing non-stoichiometric crystalline water) m.p. 371 K. IR (Nujol, ν , cm⁻¹): 1632 (imine band). UV-VIS (diffuse reflectance, nm): 255, 329, 470s h.

S3. Refinement

All H atoms were located in a difference map and refined freely [O-H = 0.98 (3) Å and C-H = 0.91 (3)-1.02 (3) Å]. Friedel pairs were merged.

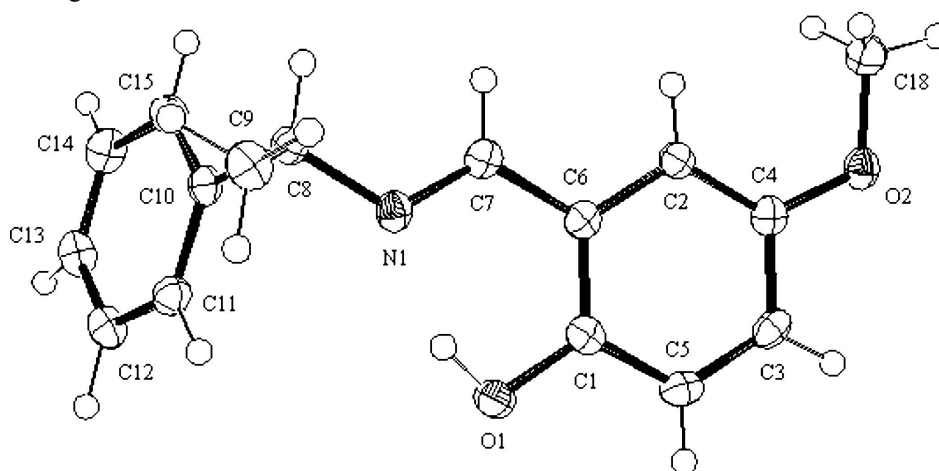


Figure 1

The molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.

(R)-4-methoxy-2-[(1-phenylethyl)iminomethyl]phenol*Crystal data*C₁₆H₁₇NO₂*M_r* = 255.31Monoclinic, *P*2₁Hall symbol: *P* 2y₁*a* = 8.270 (4) Å*b* = 5.886 (3) Å*c* = 13.920 (7) Å β = 93.254 (7)°*V* = 676.4 (6) Å³*Z* = 2*F*(000) = 272*D_x* = 1.253 Mg m⁻³Mo *K*α radiation, λ = 0.71073 Å

Cell parameters from 1657 reflections

 θ = 2.5–27.5° μ = 0.08 mm⁻¹*T* = 100 K

Plate, yellow

0.21 × 0.19 × 0.07 mm

*Data collection*Bruker SMART CCD area-detector
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

Detector resolution: 8.333 pixels mm⁻¹ φ and ω scans

Absorption correction: multi-scan

(SADABS; Bruker, 1998)

T_{min} = 0.983, *T_{max}* = 0.994

3805 measured reflections

1677 independent reflections

1454 reflections with *I* > 2σ(*I*)*R_{int}* = 0.074 θ_{\max} = 27.5°, θ_{\min} = 1.5°*h* = -10→8*k* = -7→7*l* = -17→16*Refinement*Refinement on *F*²

Least-squares matrix: full

R [*F*² > 2σ(*F*²)] = 0.042*wR*(*F*²) = 0.088*S* = 0.99

1677 reflections

240 parameters

1 restraint

Primary atom site location: structure-invariant
direct methods
Secondary atom site location: difference Fourier
map
Hydrogen site location: inferred from
neighbouring sites

All H-atom parameters refined
 $w = 1/[\sigma^2(F_o^2) + (0.038P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 0.31 \text{ e } \text{Å}^{-3}$
 $\Delta\rho_{\min} = -0.18 \text{ e } \text{Å}^{-3}$

Special details

Experimental. 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.

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.

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	−0.10235 (18)	0.3421 (3)	0.24677 (11)	0.0246 (4)
O2	−0.34502 (18)	0.0560 (3)	−0.11019 (11)	0.0236 (4)
N1	0.0495 (2)	−0.0409 (3)	0.26781 (13)	0.0209 (4)
C1	−0.1599 (2)	0.2610 (4)	0.15989 (16)	0.0204 (5)
C2	−0.2717 (3)	0.3907 (4)	0.10592 (17)	0.0235 (5)
C3	−0.3316 (2)	0.3147 (4)	0.01743 (17)	0.0214 (5)
C4	−0.2782 (2)	0.1095 (4)	−0.02039 (15)	0.0202 (5)
C5	−0.1684 (3)	−0.0231 (4)	0.03255 (16)	0.0200 (5)
C6	−0.1087 (2)	0.0500 (4)	0.12470 (15)	0.0190 (5)
C7	0.0002 (2)	−0.0964 (4)	0.18197 (16)	0.0198 (5)
C8	0.1607 (3)	−0.1916 (4)	0.32334 (16)	0.0204 (5)
C9	0.0764 (3)	−0.2731 (5)	0.41192 (19)	0.0253 (6)
C10	0.3138 (2)	−0.0565 (4)	0.34822 (15)	0.0200 (5)
C15	0.4606 (3)	−0.1240 (5)	0.31292 (16)	0.0237 (5)
C14	0.5988 (3)	0.0075 (5)	0.32986 (17)	0.0265 (6)
C13	0.5917 (3)	0.2063 (5)	0.38184 (17)	0.0269 (6)
C12	0.4471 (3)	0.2741 (5)	0.41913 (16)	0.0251 (5)
C11	0.3098 (3)	0.1428 (4)	0.40203 (16)	0.0224 (5)
C16	−0.3038 (3)	−0.1589 (5)	−0.14857 (18)	0.0255 (6)
H1	−0.041 (3)	0.216 (6)	0.2758 (19)	0.044 (9)*
H2	−0.307 (3)	0.526 (5)	0.1294 (16)	0.020 (6)*
H3	−0.408 (3)	0.398 (5)	−0.0179 (16)	0.024 (6)*
H5	−0.129 (3)	−0.164 (4)	0.0095 (14)	0.013 (6)*
H7	0.039 (3)	−0.236 (5)	0.1538 (15)	0.021 (6)*
H8	0.186 (3)	−0.326 (5)	0.2845 (16)	0.022 (6)*
H15	0.466 (3)	−0.261 (5)	0.2753 (19)	0.036 (8)*
H14	0.701 (3)	−0.044 (5)	0.3014 (16)	0.030 (7)*
H13	0.684 (3)	0.319 (6)	0.390 (2)	0.046 (8)*
H12	0.443 (3)	0.421 (5)	0.4568 (16)	0.028 (7)*

H11	0.210 (3)	0.198 (5)	0.4247 (16)	0.029 (6)*
H9A	0.045 (3)	-0.149 (5)	0.4484 (17)	0.031 (7)*
H16A	-0.330 (3)	-0.274 (5)	-0.1053 (18)	0.031 (7)*
H9B	-0.020 (3)	-0.371 (5)	0.3935 (16)	0.026 (6)*
H16B	-0.191 (3)	-0.172 (4)	-0.1610 (14)	0.014 (5)*
H9C	0.147 (3)	-0.381 (6)	0.4531 (19)	0.043 (8)*
H16C	-0.365 (3)	-0.172 (5)	-0.2090 (18)	0.027 (7)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0236 (8)	0.0249 (10)	0.0252 (9)	-0.0010 (8)	0.0002 (7)	-0.0063 (8)
O2	0.0230 (8)	0.0276 (10)	0.0198 (8)	0.0002 (7)	-0.0012 (6)	0.0021 (8)
N1	0.0171 (8)	0.0238 (11)	0.0218 (10)	-0.0012 (8)	0.0011 (7)	-0.0013 (9)
C1	0.0191 (10)	0.0217 (14)	0.0208 (12)	-0.0029 (10)	0.0046 (9)	-0.0015 (10)
C2	0.0208 (10)	0.0195 (13)	0.0306 (13)	0.0001 (10)	0.0055 (9)	-0.0011 (12)
C3	0.0144 (10)	0.0230 (13)	0.0268 (13)	0.0015 (9)	0.0023 (9)	0.0066 (11)
C4	0.0174 (10)	0.0251 (14)	0.0184 (12)	-0.0031 (9)	0.0035 (9)	0.0022 (10)
C5	0.0173 (10)	0.0210 (13)	0.0219 (12)	-0.0021 (9)	0.0033 (8)	-0.0003 (10)
C6	0.0160 (9)	0.0203 (12)	0.0209 (11)	-0.0021 (9)	0.0031 (9)	0.0001 (10)
C7	0.0155 (9)	0.0230 (13)	0.0212 (12)	-0.0017 (9)	0.0043 (8)	0.0002 (10)
C8	0.0202 (10)	0.0194 (12)	0.0215 (12)	0.0014 (9)	0.0002 (9)	-0.0014 (10)
C9	0.0233 (11)	0.0265 (14)	0.0263 (13)	-0.0046 (11)	0.0019 (10)	0.0000 (11)
C10	0.0219 (10)	0.0228 (13)	0.0149 (11)	-0.0009 (10)	-0.0015 (8)	0.0034 (10)
C15	0.0234 (11)	0.0286 (14)	0.0193 (12)	0.0033 (10)	0.0024 (9)	0.0005 (11)
C14	0.0213 (11)	0.0342 (16)	0.0242 (13)	0.0011 (10)	0.0042 (9)	0.0044 (11)
C13	0.0258 (12)	0.0322 (15)	0.0224 (13)	-0.0081 (11)	-0.0012 (10)	0.0043 (11)
C12	0.0302 (12)	0.0255 (14)	0.0192 (12)	-0.0041 (11)	-0.0014 (9)	0.0002 (11)
C11	0.0219 (11)	0.0233 (13)	0.0219 (12)	0.0021 (10)	0.0011 (9)	0.0000 (10)
C16	0.0269 (12)	0.0280 (15)	0.0217 (14)	0.0011 (11)	0.0011 (10)	-0.0009 (12)

Geometric parameters (Å, °)

O1—C1	1.361 (3)	C8—H8	0.99 (3)
O1—H1	0.98 (3)	C9—H9A	0.93 (3)
O2—C4	1.374 (3)	C9—H9B	1.00 (3)
O2—C16	1.422 (3)	C9—H9C	1.02 (3)
N1—C7	1.283 (3)	C10—C15	1.393 (3)
N1—C8	1.466 (3)	C10—C11	1.393 (3)
C1—C2	1.387 (3)	C15—C14	1.390 (4)
C1—C6	1.409 (3)	C15—H15	0.96 (3)
C2—C3	1.376 (3)	C14—C13	1.379 (4)
C2—H2	0.91 (3)	C14—H14	1.00 (2)
C3—C4	1.399 (3)	C13—C12	1.389 (3)
C3—H3	0.92 (3)	C13—H13	1.01 (3)
C4—C5	1.379 (3)	C12—C11	1.383 (3)
C5—C6	1.415 (3)	C12—H12	1.01 (3)
C5—H5	0.95 (2)	C11—H11	0.95 (3)

C6—C7	1.452 (3)	C16—H16A	0.94 (3)
C7—H7	0.97 (3)	C16—H16B	0.96 (2)
C8—C10	1.519 (3)	C16—H16C	0.96 (3)
C8—C9	1.528 (3)		
C1—O1—H1	104.5 (17)	C8—C9—H9A	110.3 (16)
C4—O2—C16	116.9 (2)	C8—C9—H9B	111.4 (13)
C7—N1—C8	119.6 (2)	H9A—C9—H9B	111 (2)
O1—C1—C2	118.5 (2)	C8—C9—H9C	112.1 (14)
O1—C1—C6	121.4 (2)	H9A—C9—H9C	110 (2)
C2—C1—C6	120.1 (2)	H9B—C9—H9C	102 (2)
C3—C2—C1	120.0 (2)	C15—C10—C11	118.5 (2)
C3—C2—H2	119.8 (16)	C15—C10—C8	120.2 (2)
C1—C2—H2	120.2 (16)	C11—C10—C8	121.22 (19)
C2—C3—C4	120.8 (2)	C14—C15—C10	120.4 (2)
C2—C3—H3	120.4 (16)	C14—C15—H15	119.8 (16)
C4—C3—H3	118.8 (16)	C10—C15—H15	119.8 (16)
O2—C4—C5	125.1 (2)	C13—C14—C15	120.2 (2)
O2—C4—C3	114.9 (2)	C13—C14—H14	121.9 (17)
C5—C4—C3	120.0 (2)	C15—C14—H14	117.9 (17)
C4—C5—C6	119.9 (2)	C14—C13—C12	120.2 (2)
C4—C5—H5	122.7 (14)	C14—C13—H13	124.3 (17)
C6—C5—H5	117.4 (14)	C12—C13—H13	115.3 (18)
C1—C6—C5	119.1 (2)	C11—C12—C13	119.4 (2)
C1—C6—C7	121.4 (2)	C11—C12—H12	121.2 (14)
C5—C6—C7	119.4 (2)	C13—C12—H12	119.4 (14)
N1—C7—C6	121.0 (2)	C12—C11—C10	121.2 (2)
N1—C7—H7	119.8 (14)	C12—C11—H11	117.8 (17)
C6—C7—H7	119.2 (14)	C10—C11—H11	120.8 (17)
N1—C8—C10	107.1 (2)	O2—C16—H16A	109.4 (17)
N1—C8—C9	108.32 (18)	O2—C16—H16B	113.2 (14)
C10—C8—C9	113.1 (2)	H16A—C16—H16B	109 (2)
N1—C8—H8	110.1 (14)	O2—C16—H16C	106.1 (17)
C10—C8—H8	110.1 (14)	H16A—C16—H16C	112 (2)
C9—C8—H8	108.1 (14)	H16B—C16—H16C	107.6 (18)
O1—C1—C2—C3	179.53 (18)	C1—C6—C7—N1	2.0 (3)
C6—C1—C2—C3	-0.6 (3)	C5—C6—C7—N1	-176.18 (18)
C1—C2—C3—C4	-1.6 (3)	C7—N1—C8—C10	120.2 (2)
C16—O2—C4—C5	3.7 (3)	C7—N1—C8—C9	-117.5 (2)
C16—O2—C4—C3	-175.42 (18)	N1—C8—C10—C15	-116.8 (2)
C2—C3—C4—O2	-178.62 (18)	C9—C8—C10—C15	124.0 (2)
C2—C3—C4—C5	2.2 (3)	N1—C8—C10—C11	59.8 (3)
O2—C4—C5—C6	-179.69 (17)	C9—C8—C10—C11	-59.5 (3)
C3—C4—C5—C6	-0.6 (3)	C11—C10—C15—C14	-1.1 (3)
O1—C1—C6—C5	-177.98 (17)	C8—C10—C15—C14	175.5 (2)
C2—C1—C6—C5	2.2 (3)	C10—C15—C14—C13	0.0 (4)
O1—C1—C6—C7	3.8 (3)	C15—C14—C13—C12	1.2 (4)

C2—C1—C6—C7	-176.03 (19)	C14—C13—C12—C11	-1.3 (4)
C4—C5—C6—C1	-1.5 (3)	C13—C12—C11—C10	0.1 (4)
C4—C5—C6—C7	176.70 (19)	C15—C10—C11—C12	1.1 (3)
C8—N1—C7—C6	-179.40 (18)	C8—C10—C11—C12	-175.5 (2)

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>
O1—H1...N1	0.97 (3)	1.72 (5)	2.589 (2)	151 (3)
C12—H12...Cg1 ⁱ	1.03 (4)	2.72 (3)	3.536 (3)	137 (3)
C16—H16C...Cg1 ⁱⁱ	0.98 (4)	2.71 (3)	3.563 (3)	149 (3)

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