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5-{2-[(2-Hydroxy-5-methylphenyl)(phenyl)methyleneamino]phenyliminomethyl}pyrrole-2-carbaldehyde

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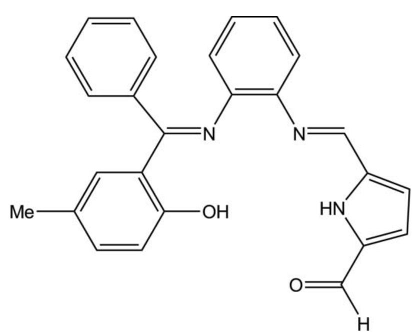
Key indicators: single-crystal X-ray study; T = 113 K; mean σ(C–C) = 0.003 Å; R factor = 0.048; wR factor = 0.130; data-to-parameter ratio = 12.9.

The title compound, $C_{26}H_{21}N_3O_2$, is an unsymmetrical tetradentate Schiff base ligand. The hydroxy group forms an intramolecular O—H···N hydrogen bond with an adjacent N atom. An intermolecular N—H···O hydrogen bond creates centrosymmetric dimers in the crystal packing.

Related literature

For background, see: Ainscough *et al.* (1995); Aruffo *et al.* (1984). For further synthetic details, see: Atkins *et al.* (1985); Miller & Olsson (1981); Olsson & Pernemalm (1979); Zhu *et al.* (2004).



Experimental

Crystal data

$C_{26}H_{21}N_3O_2$
M_r = 407.46
Triclinic, $P\bar{1}$
a = 8.8299 (18) Å
b = 9.4816 (19) Å
c = 13.130 (3) Å
α = 94.05 (3)°
β = 106.32 (3)°
γ = 94.88 (3)°
V = 1046.0 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 113 (2) K
0.22 × 0.16 × 0.12 mm

Data collection

Rigaku R-AXIS RAPID-S diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2001)
T_{min} = 0.98, T_{max} = 0.99
10760 measured reflections
3695 independent reflections
3065 reflections with $I > 2\sigma(I)$
R_{int} = 0.042

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.129
S = 1.08
3695 reflections
286 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3A···O2^{i}	0.95 (2)	1.98 (2)	2.902 (2)	164.2 (18)
O1—H1···N1	0.82	1.81	2.536 (2)	147

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

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); 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: *SHELXTL*.

The authors thank Nankai University for supporting this work.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BG2193).

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supplementary materials

Acta Cryst. (2008). E**64**, o1552 [doi:10.1107/S1600536808021922]

5-{2-[(2-Hydroxy-5-methylphenyl)(phenyl)methyleneamino]phenyliminomethyl}pyrrole-2-carbaldehyde

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Comment

Unsymmetrical Schiff base ligands have been widely investigated due to their structural versatility; specially their metal complexes have been of interest to chemists (Aruffo *et al.*, 1984; Ainscough *et al.*,1995). In the course of the synthesis of one such a complex (Zhu *et al.*, 2004; Atkins *et al.*,1985), single crystals of the title compound $C_{26}H_{21}N_3O_2$ (I) were obtained, and its crystal and molecular structure is reported here (Fig.1). An intermolecular N—H···O hydrogen bond is formed between the *H*(pyrrole) atom of one molecule and *O*(aldehyde) of an adjacent molecule (Table 1), giving raise to centrosymmetric dimers in the crystal packing, piled as columnar arrays along a, as shown in Fig. 2

Moreover, the hydroxy group is involved in an intramolecular O—H···N hydrogen bond (Table 1, Fig.1), though which atoms O1, H1, N1, C8, C1 and C2 form a six-membered ring.

Experimental

To a solution of 2-[(2-Aminophenyl)(phenyl)methyl]-4-methylphenol (0.2 mmol)(Atkins *et al.*,1985) in toluene (20 ml) was added pyrrole-2,5-dicarboxaldehyde (0.2 mmol)(Miller & Olsson, 1981; Olsso & Pernemalm, 1979) the mixture was stired and refluxed for two hours, then cooled. Rotary evaporation of solvent yielded the crude product; after chromatographic fractionating, it was recrystallized from the mixture of dichloromethane and hexane. Orange columnar crystals were obtained by evaporating the solvent at room temperature for about a week. yield: 53%, mp = 175°. Anal. for ($C_{26}H_{21}N_3O_2$), Calc. C, 76.64; H, 5.19; N, 10.31; Found: C, 76.12; H, 5.62; N, 10.19.

Refinement

The H atoms (except H3A attached to N3) were positioned geometrically and allowed to ride on their parent atoms, with C—H=0.93Å and U_{iso}(H)=1.2U_{eq}(C) for the aromatic and pyrrole ring H atoms, C—H=0.96Å, and U_{iso}(H)=1.5U_{eq}(C) for the methyl H atoms, O-H: 0.82Å, U_{iso}(H)=1.5U_{eq}(O). H3A was found in the difference Fourier and refined freely with isotropic displacement parameters.

Figures

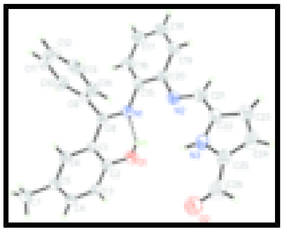

Fig. 1. The structure of the title compound with 30% displacement probability.

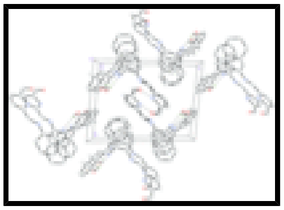

Fig. 2. Crystal packing of the title compound, showing dimers piled along a. Hydrogen bonds shown as dashed lines.

5-{2-[(2-Hydroxy-5- methylphenyl)(phenyl)methyleneamino]phenyliminomethyl}pyrrole-2-carbaldehyde

Crystal data

$C_{26}H_{21}N_3O_2$	$Z = 2$
$M_r = 407.46$	$F_{000} = 428$
Triclinic, $P\overline{1}$	$D_x = 1.294$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 8.8299$ (18) Å	Cell parameters from 3625 reflections
$b = 9.4816$ (19) Å	$\theta = 2.2–27.9°$
$c = 13.130$ (3) Å	$\mu = 0.08$ mm^{-1}
$\alpha = 94.05$ (3)°	$T = 113$ (2) K
$\beta = 106.32$ (3)°	Block, orange
$\gamma = 94.88$ (3)°	0.22 × 0.16 × 0.12 mm
$V = 1046.0$ (4) Å^3	

Data collection

Rigaku R-AXIS RAPID-S diffractometer	3695 independent reflections
Radiation source: fine-focus sealed tube	3065 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.042$
$T = 113(2)$ K	$\theta_{max} = 25.0°$
ω scans	$\theta_{min} = 1.6°$
Absorption correction: multi-scan (Crystalclear; Rigaku/MSC, 2001)	$h = -10\rightarrow10$
$T_{min} = 0.98$, $T_{max} = 0.99$	$k = -11\rightarrow11$
10760 measured reflections	$l = -15\rightarrow15$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.047$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.129$	$w = 1/[\sigma^2(F_o^2) + (0.0642P)^2 + 0.0663P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.08$	$(\Delta/\sigma)_{max} < 0.001$
3695 reflections	$\Delta\rho_{max} = 0.18$ e Å^{-3}

286 parameters	$\Delta\rho_{min} = -0.25$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 $F^2 > \sigma(F^2)$ 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}
O2	0.45524 (17)	0.34953 (15)	0.43121 (12)	0.0511 (4)
O1	0.99294 (14)	0.64418 (13)	0.90770 (11)	0.0365 (3)
H1	1.0207	0.6932	0.8657	0.055*
N1	0.98930 (16)	0.84591 (15)	0.79037 (11)	0.0272 (4)
N2	0.96097 (17)	0.77359 (15)	0.57380 (11)	0.0299 (4)
N3	0.74047 (18)	0.54096 (16)	0.44365 (12)	0.0317 (4)
C1	0.79083 (19)	0.80636 (17)	0.87844 (13)	0.0237 (4)
C2	0.8592 (2)	0.68803 (18)	0.92457 (14)	0.0280 (4)
C3	0.7899 (2)	0.61353 (18)	0.99065 (14)	0.0317 (4)
H3	0.8377	0.5384	1.0237	0.038*
C4	0.6508 (2)	0.65101 (18)	1.00712 (14)	0.0298 (4)
H4	0.6055	0.5997	1.0510	0.036*
C5	0.5756 (2)	0.76395 (18)	0.95990 (13)	0.0267 (4)
C6	0.64834 (19)	0.84052 (18)	0.89718 (13)	0.0258 (4)
H6	0.6013	0.9173	0.8663	0.031*
C7	0.4228 (2)	0.8022 (2)	0.97928 (15)	0.0343 (4)
H7A	0.4454	0.8515	1.0492	0.051*
H7B	0.3529	0.7171	0.9741	0.051*
H7C	0.3730	0.8625	0.9269	0.051*
C8	0.86574 (19)	0.88993 (17)	0.81202 (13)	0.0243 (4)
C9	0.79928 (19)	1.02221 (18)	0.77147 (13)	0.0251 (4)
C10	0.8237 (2)	1.14705 (19)	0.83785 (15)	0.0357 (5)
H10	0.8767	1.1484	0.9100	0.043*
C11	0.7691 (2)	1.2706 (2)	0.79686 (17)	0.0438 (5)
H11	0.7873	1.3548	0.8415	0.053*
C12	0.6882 (2)	1.2690 (2)	0.69028 (18)	0.0430 (5)
H12	0.6520	1.3518	0.6631	0.052*
C13	0.6611 (2)	1.1440 (2)	0.62386 (16)	0.0373 (5)
H13	0.6050	1.1424	0.5522	0.045*
C14	0.71752 (19)	1.02080 (19)	0.66395 (14)	0.0296 (4)

H14	0.7007	0.9372	0.6189	0.036*
C15	1.07804 (19)	0.92923 (18)	0.73647 (13)	0.0260 (4)
C16	1.1816 (2)	1.04669 (19)	0.79313 (15)	0.0324 (4)
H16	1.1853	1.0730	0.8634	0.039*
C17	1.2783 (2)	1.12397 (19)	0.74603 (15)	0.0345 (5)
H17	1.3471	1.2016	0.7846	0.041*
C18	1.2727 (2)	1.08574 (19)	0.64174 (15)	0.0345 (5)
H18	1.3376	1.1376	0.6097	0.041*
C19	1.1705 (2)	0.97020 (19)	0.58480 (15)	0.0324 (4)
H19	1.1664	0.9464	0.5141	0.039*
C20	1.07336 (19)	0.88838 (18)	0.63105 (14)	0.0270 (4)
C21	0.9842 (2)	0.71074 (19)	0.49084 (14)	0.0328 (4)
H21	1.0767	0.7388	0.4736	0.039*
C22	0.8739 (2)	0.59846 (18)	0.42278 (14)	0.0313 (4)
C23	0.8828 (2)	0.5293 (2)	0.32786 (15)	0.0392 (5)
H23	0.9618	0.5477	0.2949	0.047*
C24	0.7517 (2)	0.4276 (2)	0.29150 (15)	0.0407 (5)
H24	0.7272	0.3655	0.2297	0.049*
C25	0.6644 (2)	0.4354 (2)	0.36358 (14)	0.0349 (5)
C26	0.5251 (2)	0.3451 (2)	0.36340 (16)	0.0431 (5)
H26	0.4841	0.2765	0.3057	0.052*
H3A	0.692 (2)	0.574 (2)	0.4957 (16)	0.049 (6)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O2	0.0440 (9)	0.0476 (9)	0.0613 (10)	−0.0052 (7)	0.0220 (8)	−0.0130 (7)
O1	0.0350 (8)	0.0358 (8)	0.0477 (9)	0.0133 (6)	0.0212 (6)	0.0145 (6)
N1	0.0279 (8)	0.0282 (8)	0.0270 (8)	0.0030 (6)	0.0109 (6)	0.0015 (6)
N2	0.0300 (8)	0.0288 (8)	0.0301 (9)	0.0000 (6)	0.0088 (7)	0.0015 (6)
N3	0.0325 (9)	0.0312 (9)	0.0298 (9)	0.0014 (7)	0.0081 (7)	−0.0021 (7)
C1	0.0251 (9)	0.0229 (9)	0.0213 (9)	0.0005 (7)	0.0054 (7)	−0.0016 (7)
C2	0.0259 (9)	0.0267 (10)	0.0310 (10)	0.0026 (7)	0.0089 (8)	−0.0016 (7)
C3	0.0347 (10)	0.0251 (10)	0.0361 (11)	0.0044 (8)	0.0102 (8)	0.0062 (8)
C4	0.0337 (10)	0.0254 (10)	0.0300 (10)	−0.0038 (7)	0.0111 (8)	0.0015 (7)
C5	0.0259 (9)	0.0262 (9)	0.0260 (10)	−0.0016 (7)	0.0072 (7)	−0.0040 (7)
C6	0.0263 (9)	0.0248 (9)	0.0241 (9)	0.0029 (7)	0.0046 (7)	−0.0013 (7)
C7	0.0324 (10)	0.0353 (11)	0.0369 (11)	0.0031 (8)	0.0132 (8)	0.0033 (8)
C8	0.0257 (9)	0.0243 (9)	0.0208 (9)	−0.0011 (7)	0.0058 (7)	−0.0034 (7)
C9	0.0230 (9)	0.0265 (9)	0.0287 (10)	0.0012 (7)	0.0124 (7)	0.0032 (7)
C10	0.0393 (11)	0.0315 (11)	0.0366 (11)	0.0023 (8)	0.0134 (9)	−0.0014 (8)
C11	0.0491 (13)	0.0261 (11)	0.0610 (15)	0.0041 (9)	0.0250 (11)	−0.0004 (9)
C12	0.0389 (12)	0.0387 (12)	0.0639 (15)	0.0158 (9)	0.0274 (11)	0.0234 (10)
C13	0.0315 (11)	0.0471 (12)	0.0398 (11)	0.0125 (9)	0.0156 (9)	0.0159 (9)
C14	0.0245 (9)	0.0345 (10)	0.0316 (10)	0.0042 (7)	0.0105 (8)	0.0039 (8)
C15	0.0230 (9)	0.0266 (9)	0.0300 (10)	0.0062 (7)	0.0087 (7)	0.0047 (7)
C16	0.0331 (10)	0.0321 (10)	0.0304 (10)	0.0035 (8)	0.0075 (8)	0.0001 (8)
C17	0.0278 (10)	0.0330 (10)	0.0390 (12)	−0.0022 (8)	0.0059 (8)	0.0010 (8)

C18	0.0267 (10)	0.0361 (11)	0.0430 (12)	0.0007 (8)	0.0139 (9)	0.0068 (9)
C19	0.0312 (10)	0.0358 (11)	0.0323 (10)	0.0033 (8)	0.0136 (8)	0.0003 (8)
C20	0.0234 (9)	0.0274 (10)	0.0313 (10)	0.0034 (7)	0.0099 (8)	0.0019 (7)
C21	0.0310 (10)	0.0322 (11)	0.0372 (11)	0.0014 (8)	0.0135 (8)	0.0030 (8)
C22	0.0349 (10)	0.0291 (10)	0.0311 (11)	0.0042 (8)	0.0112 (8)	0.0024 (8)
C23	0.0422 (11)	0.0421 (12)	0.0354 (11)	0.0042 (9)	0.0160 (9)	−0.0019 (9)
C24	0.0433 (12)	0.0437 (12)	0.0316 (11)	0.0035 (9)	0.0082 (9)	−0.0073 (9)
C25	0.0321 (10)	0.0356 (11)	0.0308 (11)	0.0014 (8)	0.0015 (8)	−0.0043 (8)
C26	0.0355 (11)	0.0451 (12)	0.0410 (12)	−0.0003 (9)	0.0040 (10)	−0.0129 (9)

Geometric parameters (Å, °)

O2—C26	1.218 (2)	C10—H10	0.9300
O1—C2	1.354 (2)	C11—C12	1.379 (3)
O1—H1	0.8200	C11—H11	0.9300
N1—C8	1.296 (2)	C12—C13	1.382 (3)
N1—C15	1.423 (2)	C12—H12	0.9300
N2—C21	1.280 (2)	C13—C14	1.389 (2)
N2—C20	1.420 (2)	C13—H13	0.9300
N3—C22	1.362 (2)	C14—H14	0.9300
N3—C25	1.378 (2)	C15—C20	1.399 (2)
N3—H3A	0.95 (2)	C15—C16	1.399 (2)
C1—C6	1.407 (2)	C16—C17	1.380 (3)
C1—C2	1.413 (2)	C16—H16	0.9300
C1—C8	1.469 (2)	C17—C18	1.378 (2)
C2—C3	1.392 (2)	C17—H17	0.9300
C3—C4	1.376 (2)	C18—C19	1.382 (3)
C3—H3	0.9300	C18—H18	0.9300
C4—C5	1.399 (2)	C19—C20	1.398 (3)
C4—H4	0.9300	C19—H19	0.9300
C5—C6	1.386 (2)	C21—C22	1.442 (3)
C5—C7	1.510 (2)	C21—H21	0.9300
C6—H6	0.9300	C22—C23	1.392 (2)
C7—H7A	0.9600	C23—C24	1.390 (3)
C7—H7B	0.9600	C23—H23	0.9300
C7—H7C	0.9600	C24—C25	1.381 (3)
C8—C9	1.498 (2)	C24—H24	0.9300
C9—C10	1.383 (2)	C25—C26	1.436 (3)
C9—C14	1.392 (2)	C26—H26	0.9300
C10—C11	1.391 (3)		
C2—O1—H1	109.5	C13—C12—H12	120.0
C8—N1—C15	121.20 (15)	C12—C13—C14	120.07 (19)
C21—N2—C20	118.13 (15)	C12—C13—H13	120.0
C22—N3—C25	108.68 (15)	C14—C13—H13	120.0
C22—N3—H3A	128.6 (12)	C13—C14—C9	120.12 (17)
C25—N3—H3A	121.9 (12)	C13—C14—H14	119.9
C6—C1—C2	117.98 (15)	C9—C14—H14	119.9
C6—C1—C8	121.21 (16)	C20—C15—C16	119.75 (16)
C2—C1—C8	120.80 (15)	C20—C15—N1	120.96 (15)

O1—C2—C3	117.93 (16)	C16—C15—N1	119.05 (15)
O1—C2—C1	122.09 (15)	C17—C16—C15	120.85 (17)
C3—C2—C1	119.98 (15)	C17—C16—H16	119.6
C4—C3—C2	120.01 (17)	C15—C16—H16	119.6
C4—C3—H3	120.0	C18—C17—C16	119.75 (17)
C2—C3—H3	120.0	C18—C17—H17	120.1
C3—C4—C5	122.01 (16)	C16—C17—H17	120.1
C3—C4—H4	119.0	C17—C18—C19	119.95 (18)
C5—C4—H4	119.0	C17—C18—H18	120.0
C6—C5—C4	117.52 (16)	C19—C18—H18	120.0
C6—C5—C7	121.70 (16)	C18—C19—C20	121.54 (17)
C4—C5—C7	120.76 (16)	C18—C19—H19	119.2
C5—C6—C1	122.41 (16)	C20—C19—H19	119.2
C5—C6—H6	118.8	C19—C20—C15	118.12 (16)
C1—C6—H6	118.8	C19—C20—N2	123.26 (16)
C5—C7—H7A	109.5	C15—C20—N2	118.41 (15)
C5—C7—H7B	109.5	N2—C21—C22	123.21 (17)
H7A—C7—H7B	109.5	N2—C21—H21	118.4
C5—C7—H7C	109.5	C22—C21—H21	118.4
H7A—C7—H7C	109.5	N3—C22—C23	108.20 (16)
H7B—C7—H7C	109.5	N3—C22—C21	123.94 (16)
N1—C8—C1	118.17 (15)	C23—C22—C21	127.86 (18)
N1—C8—C9	121.81 (15)	C24—C23—C22	107.35 (17)
C1—C8—C9	120.02 (14)	C24—C23—H23	126.3
C10—C9—C14	119.51 (17)	C22—C23—H23	126.3
C10—C9—C8	121.20 (16)	C25—C24—C23	107.77 (17)
C14—C9—C8	119.24 (15)	C25—C24—H24	126.1
C9—C10—C11	120.09 (18)	C23—C24—H24	126.1
C9—C10—H10	120.0	N3—C25—C24	108.00 (17)
C11—C10—H10	120.0	N3—C25—C26	123.92 (17)
C12—C11—C10	120.27 (18)	C24—C25—C26	127.93 (18)
C12—C11—H11	119.9	O2—C26—C25	126.53 (18)
C10—C11—H11	119.9	O2—C26—H26	116.7
C11—C12—C13	119.92 (19)	C25—C26—H26	116.7
C11—C12—H12	120.0		

C6—C1—C2—O1	177.55 (14)	C8—C9—C14—C13	−177.17 (15)
C8—C1—C2—O1	−1.8 (2)	C8—N1—C15—C20	−109.03 (19)
C6—C1—C2—C3	−3.2 (2)	C8—N1—C15—C16	76.5 (2)
C8—C1—C2—C3	177.49 (14)	C20—C15—C16—C17	0.7 (3)
O1—C2—C3—C4	−177.69 (15)	N1—C15—C16—C17	175.21 (16)
C1—C2—C3—C4	3.0 (3)	C15—C16—C17—C18	0.3 (3)
C2—C3—C4—C5	−0.6 (3)	C16—C17—C18—C19	−0.1 (3)
C3—C4—C5—C6	−1.6 (2)	C17—C18—C19—C20	−1.1 (3)
C3—C4—C5—C7	179.84 (15)	C18—C19—C20—C15	2.1 (3)
C4—C5—C6—C1	1.4 (2)	C18—C19—C20—N2	176.60 (16)
C7—C5—C6—C1	179.91 (15)	C16—C15—C20—C19	−1.8 (3)
C2—C1—C6—C5	1.0 (2)	N1—C15—C20—C19	−176.24 (15)
C8—C1—C6—C5	−179.68 (14)	C16—C15—C20—N2	−176.62 (15)
C15—N1—C8—C1	−173.10 (14)	N1—C15—C20—N2	9.0 (2)

C15—N1—C8—C9	6.8 (2)	C21—N2—C20—C19	24.6 (3)
C6—C1—C8—N1	−174.23 (14)	C21—N2—C20—C15	−160.85 (16)
C2—C1—C8—N1	5.1 (2)	C20—N2—C21—C22	−176.30 (16)
C6—C1—C8—C9	5.9 (2)	C25—N3—C22—C23	0.3 (2)
C2—C1—C8—C9	−174.80 (14)	C25—N3—C22—C21	−179.04 (17)
N1—C8—C9—C10	−104.20 (19)	N2—C21—C22—N3	−4.9 (3)
C1—C8—C9—C10	75.7 (2)	N2—C21—C22—C23	175.81 (18)
N1—C8—C9—C14	72.9 (2)	N3—C22—C23—C24	−0.2 (2)
C1—C8—C9—C14	−107.18 (17)	C21—C22—C23—C24	179.09 (19)
C14—C9—C10—C11	−1.1 (3)	C22—C23—C24—C25	0.1 (2)
C8—C9—C10—C11	176.07 (16)	C22—N3—C25—C24	−0.3 (2)
C9—C10—C11—C12	1.0 (3)	C22—N3—C25—C26	175.55 (19)
C10—C11—C12—C13	0.1 (3)	C23—C24—C25—N3	0.1 (2)
C11—C12—C13—C14	−1.1 (3)	C23—C24—C25—C26	−175.5 (2)
C12—C13—C14—C9	1.1 (3)	N3—C25—C26—O2	0.8 (3)
C10—C9—C14—C13	0.0 (2)	C24—C25—C26—O2	175.7 (2)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3A···O2^{i}	0.95 (2)	1.98 (2)	2.902 (2)	164.2 (18)
O1—H1···N1	0.82	1.81	2.536 (2)	147

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

Fig. 1

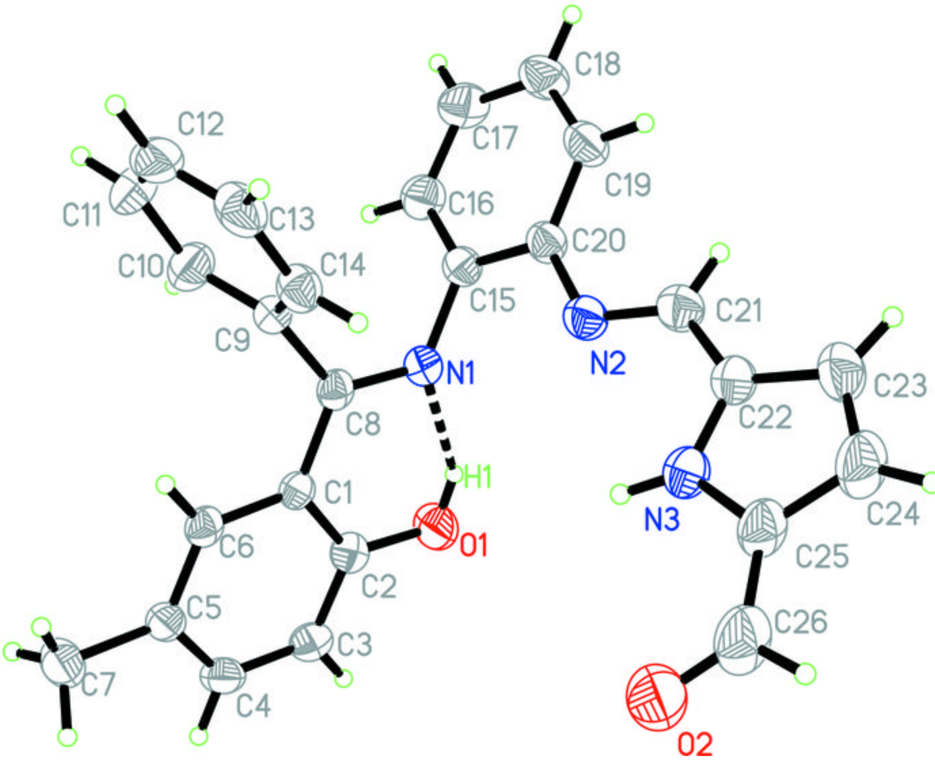
C18
C12
C17
C19
C11
C13
C16
C20
C10
C14
C21
C15
C9
N2
N1
C23
C8
C22
H1
N3
C24
C1
C6
O1
C25
C2
C5
C26
C3
C7
C4
O2

Fig. 2