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3,3′-Dimethoxy-2,2′-[*o*-phenylenebis(nitrilomethylidyne)]diphenol

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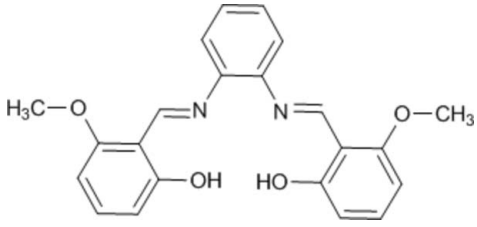
Key indicators: single-crystal X-ray study; T = 150 K; mean σ(C–C) = 0.002 Å; R factor = 0.039; wR factor = 0.111; data-to-parameter ratio = 16.0.

The title Schiff base compound, $C_{19}H_{20}N_2O_4$, was synthesized by the reaction of *o*-phenylenediamine with 6-methoxysalicylaldehyde. The central benzene ring makes dihedral angles of 2.78 (5) and 73.98 (5)° with the two terminal phenol rings. Each methoxy group is coplanar with the attached phenol ring. The crystal structure is stabilized by intramolecular O—H···N and intermolecular C—H···O hydrogen bonds.

Related literature

For general background, see: Baseer *et al.* (2000); Desai *et al.* (2001); El-Masry *et al.* (2000); Kabeer *et al.* (2001); Kuzmin *et al.* (2000); More *et al.* (2001); Singh & Dash (1988). For related structures, see: Habibi *et al.* (2007*a*,*b*).



Experimental

Crystal data

$C_{22}H_{20}N_2O_4$
M_r = 376.40
Triclinic, $P\overline{1}$
a = 8.3766 (9) Å
b = 11.1515 (11) Å
c = 11.2575 (12) Å
α = 101.848 (1)°
β = 108.359 (1)°
γ = 107.077 (1)°
V = 901.19 (16) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 150 (2) K
0.32 × 0.30 × 0.20 mm

Data collection

Bruker SMART 1K CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2007)
T_{min} = 0.970, T_{max} = 0.981
8089 measured reflections
4197 independent reflections
3504 reflections with $I > 2\sigma(I)$
R_{int} = 0.015

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.111
S = 1.04
4197 reflections
263 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.31 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
O2—H2···N1	1.00 (2)	1.65 (2)	2.5759 (14)	151.8 (19)
O3—H3···N2	0.89 (2)	1.75 (2)	2.5587 (13)	150 (2)
C8—H8*A*···O4^{i}	0.95	2.55	3.4687 (17)	164

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2005); program(s) used to refine structure: *SHELXTL*; molecular graphics: *DIAMOND* (Brandenburg, 2007); software used to prepare material for publication: *SHELXTL* and local programs.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2333).

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supplementary materials

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3,3'-Dimethoxy-2,2'-[*o*-phenylenebis(nitrilomethylidyne)]diphenol

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Comment

Schiff bases rank among the most versatile synthetic organic intermediates. They are reported to show a variety of biological activities including antifungal (Singh & Dash, 1988; More *et al.*, 2001), antibacterial (Baseer *et al.*, 2000; El-Masry *et al.*, 2000; Kabeer *et al.*, 2001) and anticancer (Kuzmin *et al.*, 2000; Desai *et al.*, 2001) among others. Recently we reported the structure of a copper(II) and nickel(II) complexes with the *N*,*N*'-bis(6-methoxysalicylidene)-1,3-diaminopropane ligand (Habibi *et al.*, 2007*a*,b)·As an extension of our investigations of Schiff base ligands and complexes, the title compound (Fig. 1) was synthesized by the reaction of *o*-phenylenediamine with 6-methoxysalicylaldehyde, and its crystal structure is reported here.

The orientations of the C2–C7 and C16–C21 benzene rings respect to the *o*-phenylenediamine unit are indicated by the dihedral angles of 73.98 (5)and 2.78 (5)°, respectively. The C2–C7 and C16–C21 benzene rings makes the dihedral angle of 73.14 (5)°. The two methoxy groups are planarly attached to the C2–C7 and C16–C21 benzene rings·The intramolecular O—H···N interactions generate S(6) ring motifs (Table 1 and Fig. 2).

Experimental

The title compound was synthesized by adding 6-methoxysalicylaldehyde (0.304 g, 2 mmol) into a solution of *o*-phenylenediamine (0.108 g, 1 mmol) in ethanol (10 ml). The mixture was refluxed with stirring for 30 min. The resultant red solution was filtered. Orange block-shaped single crystals of (I) suitable for X-ray structure determination were formed after 3 days of slow evaporation of the solvent at room temperature.

Refinement

Hydroxy H atoms were located in a difference Fourier map and refined isotropically. Methyl H atoms were placed in calculated positions with C—H = 0.98 Å and torsion angles were refined with U_{iso}(H) = 1.5U_{eq}(C). Aromatic H atoms were positioned geometrically and allowed to ride on their parent atoms with C—H = 0.95 Å, U_{iso}(H) = 1.2U_{eq}(C).

Figures

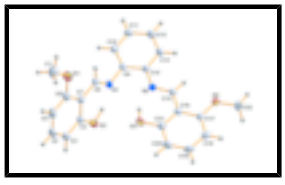

Fig. 1. The molecular structure of (I), showing 50% probability displacement ellipsoids and the atomic numbering.

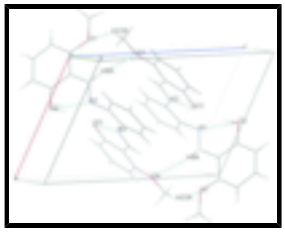

Fig. 2. The crystal packing of (I), hydrogen bonds were drawn as dash lines.

3,3'-Dimethoxy-2,2'-[1,2-phenylenebis(nitrilomethylidyne)]diphenol

Crystal data

$C_{22}H_{20}N_2O_4$	$Z = 2$
$M_r = 376.40$	$F_{000} = 396$
Triclinic, $P\overline{1}$	$D_x = 1.387$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 8.3766$ (9) Å	Cell parameters from 5073 reflections
$b = 11.1515$ (11) Å	$\theta = 2.3$–28.3°
$c = 11.2575$ (12) Å	$\mu = 0.10$ mm^{-1}
$\alpha = 101.848$ (1)°	$T = 150$ (2) K
$\beta = 108.359$ (1)°	Block, orange
$\gamma = 107.077$ (1)°	0.32 × 0.30 × 0.20 mm
$V = 901.19$ (16) Å^3	

Data collection

Bruker SMART 1K CCD diffractometer	4197 independent reflections
Radiation source: sealed tube	3504 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.015$
$T = 150$(2) K	$\theta_{max} = 28.3^\circ$
thin–slice ω scans	$\theta_{min} = 2.0^\circ$
Absorption correction: multi-scan (SADABS; Sheldrick, 2007)	$h = -11 \rightarrow 11$
$T_{min} = 0.970$, $T_{max} = 0.981$	$k = -14 \rightarrow 14$
8089 measured reflections	$l = -14 \rightarrow 15$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.039$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.111$	$w = 1/[\sigma^2(F_o^2) + (0.0546P)^2 + 0.2872P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.04$	$(\Delta/\sigma)_{max} < 0.001$

4197 reflections	$\Delta\rho_{max} = 0.31$ e Å^{-3}
263 parameters	$\Delta\rho_{min} = -0.18$ 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 $F^2 > 2\text{sigma}(F^2)$ 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}
O1	−0.13493 (13)	0.19435 (9)	0.03338 (10)	0.0361 (2)
O2	0.41326 (13)	0.32229 (10)	−0.03430 (10)	0.0335 (2)
H2	0.432 (3)	0.397 (2)	0.042 (2)	0.069 (6)*
O3	0.55943 (13)	0.25477 (9)	0.26963 (9)	0.0335 (2)
H3	0.547 (3)	0.332 (2)	0.284 (2)	0.070 (6)*
O4	1.01314 (12)	0.49961 (8)	0.70540 (8)	0.0257 (2)
N1	0.36681 (13)	0.46636 (10)	0.15216 (10)	0.0225 (2)
N2	0.61616 (14)	0.49466 (9)	0.38789 (10)	0.0229 (2)
C1	−0.31728 (19)	0.10418 (15)	−0.00296 (16)	0.0402 (4)
H1A	−0.3665	0.1384	0.0586	0.060*
H1B	−0.3169	0.0172	0.0008	0.060*
H1C	−0.3933	0.0951	−0.0932	0.060*
C2	0.24429 (17)	0.23396 (12)	−0.06730 (12)	0.0260 (3)
C3	0.1757 (2)	0.11749 (14)	−0.17425 (13)	0.0333 (3)
H3A	0.2470	0.1020	−0.2221	0.040*
C4	0.0033 (2)	0.02529 (13)	−0.20961 (14)	0.0370 (3)
H4A	−0.0414	−0.0546	−0.2812	0.044*
C5	−0.10797 (19)	0.04491 (13)	−0.14405 (14)	0.0342 (3)
H5A	−0.2267	−0.0200	−0.1708	0.041*
C6	−0.04092 (17)	0.16164 (12)	−0.03873 (13)	0.0273 (3)
C7	0.13665 (16)	0.25797 (11)	0.00215 (11)	0.0231 (2)
C8	0.20536 (16)	0.37949 (11)	0.11280 (11)	0.0218 (2)
H8A	0.1294	0.3946	0.1565	0.026*
C9	0.43040 (15)	0.58591 (11)	0.25858 (11)	0.0198 (2)
C10	0.36779 (17)	0.68650 (12)	0.24104 (12)	0.0249 (3)
H10A	0.2758	0.6735	0.1588	0.030*
C11	0.44001 (18)	0.80535 (12)	0.34372 (13)	0.0266 (3)
H11A	0.3969	0.8737	0.3319	0.032*

C12	0.57513 (17)	0.82492 (12)	0.46385 (13)	0.0268 (3)
H12A	0.6250	0.9069	0.5337	0.032*
C13	0.63754 (17)	0.72499 (12)	0.48213 (12)	0.0259 (3)
H13A	0.7293	0.7387	0.5648	0.031*
C14	0.56646 (15)	0.60432 (11)	0.37985 (11)	0.0201 (2)
C15	0.74570 (15)	0.49796 (11)	0.48910 (11)	0.0204 (2)
H15A	0.8125	0.5768	0.5636	0.024*
C16	0.78987 (16)	0.38175 (11)	0.48972 (12)	0.0208 (2)
C17	0.92887 (16)	0.38330 (12)	0.60199 (12)	0.0219 (2)
C18	0.97267 (17)	0.27272 (13)	0.60344 (13)	0.0276 (3)
H18A	1.0656	0.2743	0.6793	0.033*
C19	0.87784 (19)	0.15936 (13)	0.49159 (14)	0.0318 (3)
H19A	0.9081	0.0837	0.4919	0.038*
C20	0.74174 (19)	0.15375 (13)	0.38064 (14)	0.0320 (3)
H20A	0.6793	0.0751	0.3057	0.038*
C21	0.69577 (17)	0.26434 (12)	0.37869 (12)	0.0254 (3)
C22	1.14988 (18)	0.50459 (14)	0.82323 (13)	0.0320 (3)
H22A	1.2030	0.5937	0.8885	0.048*
H22B	1.2456	0.4841	0.8019	0.048*
H22C	1.0946	0.4394	0.8600	0.048*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0267 (5)	0.0295 (5)	0.0411 (6)	0.0010 (4)	0.0136 (4)	0.0044 (4)
O2	0.0281 (5)	0.0360 (5)	0.0310 (5)	0.0104 (4)	0.0130 (4)	0.0009 (4)
O3	0.0389 (5)	0.0245 (5)	0.0262 (5)	0.0141 (4)	0.0025 (4)	0.0009 (4)
O4	0.0261 (4)	0.0257 (4)	0.0222 (4)	0.0112 (4)	0.0052 (3)	0.0073 (3)
N1	0.0227 (5)	0.0216 (5)	0.0197 (5)	0.0082 (4)	0.0066 (4)	0.0034 (4)
N2	0.0259 (5)	0.0189 (5)	0.0229 (5)	0.0100 (4)	0.0079 (4)	0.0057 (4)
C1	0.0258 (7)	0.0371 (8)	0.0475 (9)	0.0011 (6)	0.0104 (6)	0.0168 (7)
C2	0.0265 (6)	0.0259 (6)	0.0226 (6)	0.0130 (5)	0.0050 (5)	0.0057 (5)
C3	0.0387 (7)	0.0321 (7)	0.0255 (6)	0.0203 (6)	0.0070 (5)	0.0019 (5)
C4	0.0428 (8)	0.0250 (6)	0.0280 (7)	0.0150 (6)	0.0002 (6)	−0.0018 (5)
C5	0.0304 (7)	0.0221 (6)	0.0331 (7)	0.0048 (5)	−0.0008 (5)	0.0046 (5)
C6	0.0265 (6)	0.0229 (6)	0.0267 (6)	0.0082 (5)	0.0047 (5)	0.0081 (5)
C7	0.0242 (6)	0.0203 (5)	0.0213 (5)	0.0091 (5)	0.0047 (5)	0.0066 (4)
C8	0.0222 (5)	0.0229 (6)	0.0202 (5)	0.0099 (4)	0.0070 (4)	0.0077 (4)
C9	0.0190 (5)	0.0190 (5)	0.0204 (5)	0.0057 (4)	0.0091 (4)	0.0047 (4)
C10	0.0254 (6)	0.0276 (6)	0.0241 (6)	0.0130 (5)	0.0092 (5)	0.0101 (5)
C11	0.0313 (6)	0.0216 (6)	0.0336 (7)	0.0141 (5)	0.0163 (5)	0.0114 (5)
C12	0.0286 (6)	0.0174 (5)	0.0296 (6)	0.0071 (5)	0.0109 (5)	0.0021 (5)
C13	0.0248 (6)	0.0212 (6)	0.0235 (6)	0.0073 (5)	0.0040 (5)	0.0021 (5)
C14	0.0206 (5)	0.0167 (5)	0.0221 (5)	0.0068 (4)	0.0086 (4)	0.0052 (4)
C15	0.0215 (5)	0.0183 (5)	0.0209 (5)	0.0069 (4)	0.0094 (4)	0.0052 (4)
C16	0.0224 (5)	0.0196 (5)	0.0234 (6)	0.0089 (4)	0.0117 (5)	0.0079 (4)
C17	0.0214 (5)	0.0225 (6)	0.0248 (6)	0.0085 (4)	0.0118 (5)	0.0095 (5)
C18	0.0268 (6)	0.0301 (6)	0.0334 (7)	0.0157 (5)	0.0136 (5)	0.0158 (5)

C19	0.0371 (7)	0.0253 (6)	0.0429 (8)	0.0194 (5)	0.0200 (6)	0.0137 (6)
C20	0.0384 (7)	0.0212 (6)	0.0344 (7)	0.0137 (5)	0.0134 (6)	0.0039 (5)
C21	0.0280 (6)	0.0219 (6)	0.0254 (6)	0.0105 (5)	0.0100 (5)	0.0061 (5)
C22	0.0303 (7)	0.0388 (7)	0.0244 (6)	0.0165 (6)	0.0052 (5)	0.0098 (5)

Geometric parameters (Å, °)

O1—C1	1.4307 (16)	C8—H8A	0.9500
O1—C6	1.3646 (17)	C9—C10	1.3941 (16)
O2—H2	1.00 (2)	C9—C14	1.4043 (16)
O2—C2	1.3458 (16)	C10—H10A	0.9500
O3—H3	0.89 (2)	C10—C11	1.3850 (17)
O3—C21	1.3470 (15)	C11—H11A	0.9500
O4—C17	1.3639 (14)	C11—C12	1.3882 (18)
O4—C22	1.4318 (15)	C12—H12A	0.9500
N1—C8	1.2809 (15)	C12—C13	1.3878 (17)
N1—C9	1.4218 (14)	C13—H13A	0.9500
N2—C14	1.4133 (14)	C13—C14	1.3973 (16)
N2—C15	1.2874 (15)	C15—H15A	0.9500
C1—H1A	0.9800	C15—C16	1.4491 (15)
C1—H1B	0.9800	C16—C17	1.4162 (16)
C1—H1C	0.9800	C16—C21	1.4140 (16)
C2—C3	1.3965 (17)	C17—C18	1.3877 (16)
C2—C7	1.4127 (18)	C18—H18A	0.9500
C3—H3A	0.9500	C18—C19	1.3932 (19)
C3—C4	1.378 (2)	C19—H19A	0.9500
C4—H4A	0.9500	C19—C20	1.376 (2)
C4—C5	1.396 (2)	C20—H20A	0.9500
C5—H5A	0.9500	C20—C21	1.3979 (17)
C5—C6	1.3903 (18)	C22—H22A	0.9800
C6—C7	1.4162 (17)	C22—H22B	0.9800
C7—C8	1.4548 (16)	C22—H22C	0.9800
C1—O1—C6	118.19 (11)	C10—C11—H11A	119.9
H2—O2—C2	104.6 (12)	C10—C11—C12	120.24 (11)
H3—O3—C21	107.0 (14)	H11A—C11—C12	119.9
C17—O4—C22	117.29 (10)	C11—C12—H12A	119.9
C8—N1—C9	120.25 (10)	C11—C12—C13	120.15 (11)
C14—N2—C15	123.35 (10)	H12A—C12—C13	119.9
O1—C1—H1A	109.5	C12—C13—H13A	119.7
O1—C1—H1B	109.5	C12—C13—C14	120.52 (11)
O1—C1—H1C	109.5	H13A—C13—C14	119.7
H1A—C1—H1B	109.5	N2—C14—C9	115.63 (10)
H1A—C1—H1C	109.5	N2—C14—C13	125.54 (10)
H1B—C1—H1C	109.5	C9—C14—C13	118.80 (10)
O2—C2—C3	118.18 (12)	N2—C15—H15A	119.9
O2—C2—C7	121.52 (11)	N2—C15—C16	120.21 (10)
C3—C2—C7	120.29 (12)	H15A—C15—C16	119.9
C2—C3—H3A	120.4	C15—C16—C17	120.61 (10)
C2—C3—C4	119.26 (13)	C15—C16—C21	121.00 (11)

H3A—C3—C4	120.4	C17—C16—C21	118.39 (10)
C3—C4—H4A	118.8	O4—C17—C16	115.11 (10)
C3—C4—C5	122.41 (12)	O4—C17—C18	123.82 (11)
H4A—C4—C5	118.8	C16—C17—C18	121.07 (11)
C4—C5—H5A	120.8	C17—C18—H18A	120.6
C4—C5—C6	118.42 (13)	C17—C18—C19	118.77 (12)
H5A—C5—C6	120.8	H18A—C18—C19	120.6
O1—C6—C5	124.72 (12)	C18—C19—H19A	119.0
O1—C6—C7	114.34 (11)	C18—C19—C20	121.96 (12)
C5—C6—C7	120.94 (13)	H19A—C19—C20	119.0
C2—C7—C6	118.66 (11)	C19—C20—H20A	120.2
C2—C7—C8	120.96 (11)	C19—C20—C21	119.66 (12)
C6—C7—C8	120.38 (11)	H20A—C20—C21	120.2
N1—C8—C7	120.98 (11)	O3—C21—C16	121.63 (11)
N1—C8—H8A	119.5	O3—C21—C20	118.22 (11)
C7—C8—H8A	119.5	C16—C21—C20	120.15 (11)
N1—C9—C10	120.92 (10)	O4—C22—H22A	109.5
N1—C9—C14	118.57 (10)	O4—C22—H22B	109.5
C10—C9—C14	120.40 (10)	O4—C22—H22C	109.5
C9—C10—H10A	120.1	H22A—C22—H22B	109.5
C9—C10—C11	119.88 (11)	H22A—C22—H22C	109.5
H10A—C10—C11	120.1	H22B—C22—H22C	109.5
O2—C2—C3—C4	179.74 (12)	C12—C13—C14—C9	−0.25 (18)
C7—C2—C3—C4	−1.21 (19)	N1—C9—C14—N2	−5.56 (15)
C2—C3—C4—C5	1.4 (2)	N1—C9—C14—C13	176.05 (10)
C3—C4—C5—C6	−0.4 (2)	C10—C9—C14—N2	178.37 (10)
C1—O1—C6—C5	−1.49 (19)	C10—C9—C14—C13	−0.01 (17)
C1—O1—C6—C7	178.56 (11)	C15—N2—C14—C9	175.83 (11)
C4—C5—C6—O1	179.44 (12)	C15—N2—C14—C13	−5.91 (19)
C4—C5—C6—C7	−0.61 (19)	C14—N2—C15—C16	−179.49 (10)
O2—C2—C7—C6	179.21 (11)	N2—C15—C16—C17	−178.30 (11)
O2—C2—C7—C8	−0.27 (18)	N2—C15—C16—C21	1.73 (17)
C3—C2—C7—C6	0.20 (18)	C22—O4—C17—C16	177.64 (10)
C3—C2—C7—C8	−179.29 (11)	C22—O4—C17—C18	−2.32 (17)
O1—C6—C7—C2	−179.32 (11)	C15—C16—C17—O4	0.26 (16)
O1—C6—C7—C8	0.17 (16)	C15—C16—C17—C18	−179.77 (11)
C5—C6—C7—C2	0.72 (18)	C21—C16—C17—O4	−179.77 (10)
C5—C6—C7—C8	−179.79 (11)	C21—C16—C17—C18	0.20 (17)
C9—N1—C8—C7	178.62 (10)	O4—C17—C18—C19	−179.67 (11)
C2—C7—C8—N1	−1.70 (17)	C16—C17—C18—C19	0.37 (18)
C6—C7—C8—N1	178.82 (11)	C17—C18—C19—C20	−0.5 (2)
C8—N1—C9—C10	−73.58 (15)	C18—C19—C20—C21	0.0 (2)
C8—N1—C9—C14	110.38 (13)	C19—C20—C21—O3	−178.67 (12)
N1—C9—C10—C11	−175.99 (11)	C19—C20—C21—C16	0.6 (2)
C14—C9—C10—C11	−0.02 (17)	C15—C16—C21—O3	−1.47 (18)
C9—C10—C11—C12	0.30 (18)	C15—C16—C21—C20	179.29 (11)
C10—C11—C12—C13	−0.56 (19)	C17—C16—C21—O3	178.56 (11)
C11—C12—C13—C14	0.53 (19)	C17—C16—C21—C20	−0.68 (18)
C12—C13—C14—N2	−178.45 (11)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···N1	1.00 (2)	1.65 (2)	2.5759 (14)	151.8 (19)
O3—H3···N2	0.89 (2)	1.75 (2)	2.5587 (13)	150 (2)
C8—H8A···O4^{i}	0.95	2.55	3.4687 (17)	164

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

Fig. 1

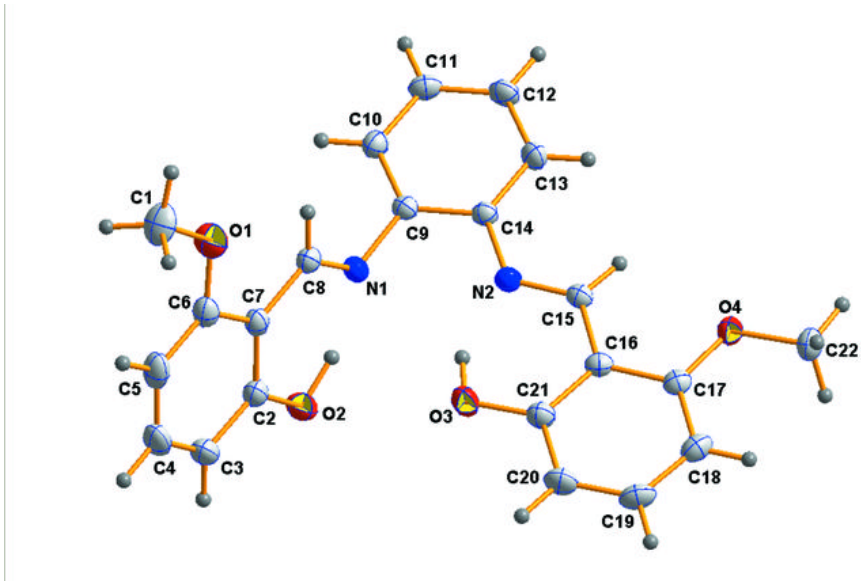
C11
C12
C10
C13
C1
O1
C9
C14
C8
N1
N2
C6
C7
C15
O4
C16
C22
C5
C21
C17
O3
C2
O2
C4
C3
C20
C18
C19

Fig. 2