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5,5′-Dimethoxy-2,2′-[1,2-phenylenebis(nitrilomethylidyne)]diphenol

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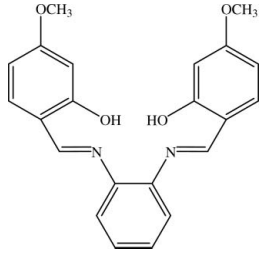
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.004 Å; R factor = 0.053; wR factor = 0.173; data-to-parameter ratio = 12.4.

The title compound, $C_{22}H_{20}N_2O_4$, is a Schiff base ligand. The dihedral angles between the central and two outer benzene rings are 2.20 (12) and 58.29 (12)°. Two O—H···N intramolecular hydrogen bonds involving the two hydroxy groups generate S(6) ring motifs. In the crystal structure, molecules are stacked approximately along the a axis and are linked by weak intermolecular C—H···O interactions. The crystal structure is stabilized by intramolecular O—H···N hydrogen bonds, weak C—H···O intermolecular interactions and C—H···π interactions.

Related literature

For related literature on hydrogen-bond motifs, see: Bernstein *et al.* (1995). For related structures, see: Eltayeb, Teoh, Chantrapromma *et al.* (2007*a*,*b*); Eltayeb, Teoh, Teh *et al.* (2007*a*,*b*). For related literature on pharmacological activities and applications, see: Dao *et al.* (2000); Karthikeyan *et al.* (2006); Sriram *et al.* (2006); Eltayeb & Ahmed (2005*a*,*b*). For related literature on bond lengths, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{22}H_{20}N_2O_4$
M_r = 376.40
Monoclinic, $P2_1/c$
a = 6.2038 (3) Å
b = 17.8512 (8) Å
c = 16.6216 (9) Å
β = 91.072 (3)°
V = 1840.44 (16) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 100.0 (1) K
0.56 × 0.09 × 0.07 mm

Data collection

Bruker SMART APEX II CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.949, T_{max} = 0.994
13290 measured reflections
3243 independent reflections
2216 reflections with $I > 2\sigma(I)$
R_{int} = 0.065

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.173
S = 1.10
3243 reflections
262 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1*O1*···N1	0.87 (3)	1.83 (4)	2.615 (3)	149 (3)
O3—H1*O3*···N2	1.03 (2)	1.61 (2)	2.555 (3)	150 (2)
C7—H7*A*···O3^{i}	0.93	2.44	3.283 (3)	150
C10—H10*A*···O2^{ii}	0.93	2.57	3.362 (3)	143
C12—H12*A*···*Cg*1^{iii}	0.93	2.80	3.614 (3)	147
C21—H21*A*···*Cg*2^{iv}	0.96	2.56	3.412 (3)	149
C22—H22*A*···*Cg*1^{v}	0.96	2.68	3.396 (3)	132

Symmetry codes: (i) $x-1, y, z$; (ii) $-x-1, y-\frac{1}{2}, -z+\frac{3}{2}$; (iii) $x, -y-\frac{1}{2}, z-\frac{1}{2}$; (iv) $-x, y+\frac{1}{2}, -z+\frac{3}{2}$; (v) $-x+1, -y+1, -z+2$.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2005); program(s) used to solve structure: *SHELXTL* (Sheldrick, 1998); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: OM2130).

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supplementary materials

Acta Cryst. (2007). E**63**, o3094-o3095 [**doi:10.1107/S1600536807026141**]

5,5'-Dimethoxy-2,2'-[1,2-phenylenebis(nitrilomethylidyne)]diphenol

N. E. Eltayeb, S. G. Teoh, S. Chantrapromma, H.-K. Fun and K. Ibrahim

Comment

Schiff base compounds have received much attention because of their potential applications. Some of these compounds exhibit various pharmacological activities, such as anticancer (Dao *et al.*, 2000), anti-HIV (Sriram *et al.*, 2006), antibacterial and antifungal (Karthikeyan *et al.*, 2006) properties. In addition, some of them may be used as analytical reagents for the determination of trace elements (Eltayeb & Ahmed, 2005*a*,b). Recently we have reported the crystal structures of 2,2'-[1,2-phenylenebis(nitrilomethylidyne)]bis(5-methylphenol) (Eltayeb, Teoh, Chantrapromma *et al.*, 2007*a*) and 6,6'-Dimethyl-2,2'-[1,2-phenylenebis(nitrilomethylidyne)]diphenol (Eltayeb, Teoh, Chantrapromma *et al.*, 2007*b*). As an extension of our investigations of Schiff base ligands and their complexes, the title compound was synthesized by the reaction of *o*-phenylenediamine and 4-methoxysalicylaldehyde, and its crystal structure is reported here.

In the structure of the title compound, the C15–C20 benzene ring is almost planar with the *o*-phenylaniline as indicated by the dihedral angle between the C8–C13 and C15–C20 benzene rings being 2.20 (12)° and the torsion angle C13/N2/C14/C15 = 178.2 (2)°. The C1–C6 benzene ring makes the dihedral angles of 58.29 (12)° and 57.60 (12)° with C8–C13 and C15–C20 benzene rings, respectively and the torsion angle C8/N1/C7/C6 is −178.8 (2)°. The two methoxy groups are slightly deviated from the mean planes of C1–C6 and C15–C20 benzene rings with the torsion angles C21/O2/C3/C2 = 5.5 (4)° and C22/O4/C18/C19 = −5.8 (4)°. The two intramolecular hydrogen bonds, O1—H1O1···N1 and O3—H1O3···N2 generate S(6) ring motifs (Bernstein *et al.*, 1995). Bond lengths and angles are in normal ranges (Allen *et al.*, 1987) and comparable to those in related structures (Eltayeb, Teoh, Chantrapromma *et al.*, 2007*a*; 2007*b*; Eltayeb, Teoh, Teh *et al.*, 2007*a*; 2007*b*).

In the crystal, the molecules are stacked approximately along the *a* axis and are linked by weak C—H···O intermolecular interactions (Table 1). The crystal is stabilized by O—H···N intramolecular hydrogen bonds, weak C—H···O intermolecular interactions and C—H···π interactions (Table 1); Cg_1 and Cg_2 are the centroids of C1–C6 and C8–C13 benzene rings, respectively.

Experimental

The title compound was synthesized by adding 4-methoxysalicylaldehyde (0.608 g, 4 mmol) into a solution of *o*-phenylenediamine (0.216 g, 2 mmol) in ethanol 95% (20 ml). The mixture was refluxed with stirring for half an hour. The resultant yellow solution was filtered. Yellow needle-shaped single crystals suitable for *x*-ray structure determination were formed after one week of slow evaporation of the solvent at room temperature.

Refinement

Hydroxyl H atoms were located from the difference map and isotropically refined. The O—H distance was restrainted to be 1.02 Å. The remaining H atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H distances in the range 0.93–0.96 Å. The U_{iso} values were constrained to be $1.5U_{eq}$ of the carrier atom for methyl H atoms and $1.2U_{eq}$ for the remaining H atoms. A rotating group model was used for the methyl groups.

Figures

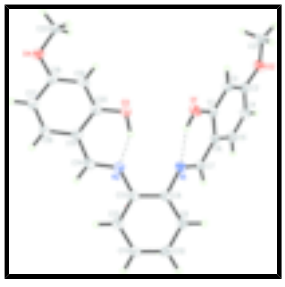

Fig. 1. The asymmetric unit, showing 50% probability displacement ellipsoids and the atomic numbering. Hydrogen bonds were drawn as dashed lines.

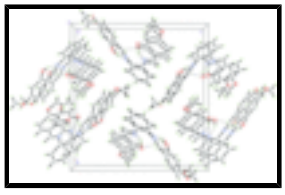

Fig. 2. The crystal packing, viewed along the *a* axis. Hydrogen bonds were drawn as dashed lines.

5,5'-Dimethoxy-2,2'-[1,2-phenylenebis(nitrilomethylidyne)]diphenol

Crystal data

$C_{22}H_{20}N_2O_4$	F_{000} = 792
M_r = 376.40	D_x = 1.358 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 3248 reflections
a = 6.2038 (3) Å	θ = 2.3–25.0º
b = 17.8512 (8) Å	μ = 0.09 mm^{-1}
c = 16.6216 (9) Å	T = 100.0 (1) K
β = 91.072 (3)º	Needle, yellow
V = 1840.44 (16) Å^3	0.56 × 0.09 × 0.07 mm
Z = 4	

Data collection

Bruker SMART APEX II CCD area-detector diffractometer	3243 independent reflections
Radiation source: fine-focus sealed tube	2216 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.065
Detector resolution: 8.33 pixels mm^{-1}	θ_{max} = 25.0º
T = 100.0(1) K	θ_{min} = 2.3º
ω scans	h = −7→7
Absorption correction: multi-scan (SADABS; Bruker, 2005)	k = −21→19
T_{min} = 0.949, T_{max} = 0.994	l = −19→17
13290 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.053$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.173$	$w = 1/[\sigma^2(F_o^2) + (0.0933P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.10$	$(\Delta/\sigma)_{max} < 0.001$
3243 reflections	$\Delta\rho_{max} = 0.33$ e Å^{-3}
262 parameters	$\Delta\rho_{min} = -0.40$ e Å^{-3}
1 restraint	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

Special details

Experimental. The low-temparture data was collected with the Oxford Cyrosystem Cobra low-temperature attachment.

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 $F^2 > 2$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	0.0703 (3)	0.32653 (11)	0.80217 (12)	0.0248 (5)
O2	−0.0700 (3)	0.55094 (10)	0.65403 (12)	0.0286 (5)
O3	0.2304 (3)	0.35378 (10)	0.98638 (11)	0.0228 (5)
H1O3	0.105 (3)	0.3163 (13)	0.9890 (18)	0.034*
O4	0.8395 (3)	0.41639 (10)	1.15245 (11)	0.0263 (5)
N1	−0.2356 (4)	0.27947 (12)	0.89576 (13)	0.0220 (5)
N2	−0.0249 (3)	0.25266 (11)	1.03707 (13)	0.0195 (5)
C1	−0.0650 (4)	0.38340 (14)	0.78190 (15)	0.0202 (6)
C2	0.0077 (4)	0.43688 (14)	0.72876 (15)	0.0201 (6)
H2A	0.1450	0.4330	0.7076	0.024*
C3	−0.1249 (4)	0.49629 (15)	0.70726 (16)	0.0232 (6)
C4	−0.3302 (5)	0.50314 (15)	0.73896 (16)	0.0252 (6)
H4A	−0.4168	0.5439	0.7254	0.030*
C5	−0.4034 (4)	0.44916 (15)	0.79042 (16)	0.0243 (6)
H5A	−0.5412	0.4535	0.8110	0.029*

C6	−0.2752 (4)	0.38736 (14)	0.81284 (15)	0.0203 (6)
C7	−0.3570 (4)	0.33203 (14)	0.86776 (16)	0.0214 (6)
H7A	−0.5002	0.3345	0.8832	0.026*
C8	−0.3254 (4)	0.22534 (14)	0.94862 (15)	0.0198 (6)
C9	−0.5118 (4)	0.18563 (14)	0.92858 (17)	0.0240 (6)
H9A	−0.5874	0.1965	0.8812	0.029*
C10	−0.5849 (4)	0.12966 (16)	0.97942 (17)	0.0258 (7)
H10A	−0.7090	0.1029	0.9659	0.031*
C11	−0.4735 (5)	0.11399 (15)	1.04981 (17)	0.0261 (7)
H11A	−0.5217	0.0760	1.0832	0.031*
C12	−0.2898 (4)	0.15427 (14)	1.07156 (17)	0.0243 (6)
H12A	−0.2186	0.1443	1.1201	0.029*
C13	−0.2122 (4)	0.20983 (14)	1.02039 (15)	0.0203 (6)
C14	0.0948 (4)	0.24777 (14)	1.10232 (16)	0.0223 (6)
H14A	0.0551	0.2148	1.1427	0.027*
C15	0.2837 (4)	0.29153 (14)	1.11309 (15)	0.0196 (6)
C16	0.4149 (4)	0.28349 (15)	1.18253 (15)	0.0225 (6)
H16A	0.3752	0.2493	1.2218	0.027*
C17	0.5979 (5)	0.32428 (14)	1.19388 (17)	0.0237 (6)
H17A	0.6838	0.3173	1.2397	0.028*
C18	0.6564 (4)	0.37763 (14)	1.13482 (16)	0.0212 (6)
C19	0.5320 (4)	0.38755 (14)	1.06639 (16)	0.0208 (6)
H19A	0.5721	0.4232	1.0287	0.025*
C20	0.3453 (4)	0.34473 (14)	1.05253 (15)	0.0199 (6)
C21	0.1296 (5)	0.54218 (18)	0.6133 (2)	0.0395 (8)
H21A	0.1471	0.5826	0.5759	0.059*
H21B	0.1290	0.4954	0.5847	0.059*
H21C	0.2467	0.5426	0.6518	0.059*
C22	0.9184 (5)	0.46624 (15)	1.09219 (17)	0.0259 (7)
H22A	1.0582	0.4845	1.1084	0.039*
H22B	0.8209	0.5077	1.0858	0.039*
H22C	0.9289	0.4400	1.0420	0.039*
H1O1	0.005 (6)	0.2990 (19)	0.837 (2)	0.052 (11)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0248 (11)	0.0254 (11)	0.0245 (11)	0.0065 (9)	0.0051 (9)	0.0069 (9)
O2	0.0292 (11)	0.0256 (11)	0.0309 (11)	−0.0004 (8)	0.0014 (9)	0.0105 (8)
O3	0.0213 (10)	0.0253 (11)	0.0219 (10)	−0.0029 (8)	0.0004 (8)	0.0020 (8)
O4	0.0249 (11)	0.0268 (11)	0.0272 (11)	−0.0061 (9)	0.0005 (8)	−0.0013 (8)
N1	0.0262 (13)	0.0227 (12)	0.0173 (12)	−0.0010 (10)	0.0029 (10)	−0.0014 (9)
N2	0.0187 (12)	0.0174 (12)	0.0226 (12)	0.0009 (9)	0.0024 (9)	−0.0019 (9)
C1	0.0233 (15)	0.0204 (15)	0.0167 (14)	0.0018 (11)	−0.0013 (11)	−0.0037 (11)
C2	0.0173 (14)	0.0243 (15)	0.0188 (14)	0.0012 (11)	0.0031 (11)	−0.0016 (11)
C3	0.0267 (16)	0.0216 (15)	0.0213 (14)	−0.0036 (12)	−0.0015 (12)	−0.0003 (11)
C4	0.0259 (16)	0.0215 (15)	0.0282 (15)	0.0048 (12)	−0.0020 (12)	0.0005 (12)
C5	0.0201 (14)	0.0286 (16)	0.0243 (15)	0.0040 (12)	0.0018 (12)	−0.0031 (12)

C6	0.0221 (15)	0.0216 (15)	0.0171 (13)	0.0001 (11)	0.0003 (11)	−0.0017 (11)
C7	0.0184 (14)	0.0250 (15)	0.0209 (14)	−0.0022 (12)	0.0014 (11)	−0.0043 (11)
C8	0.0196 (14)	0.0198 (14)	0.0200 (14)	0.0020 (11)	0.0065 (11)	−0.0026 (11)
C9	0.0238 (15)	0.0273 (16)	0.0209 (14)	0.0005 (12)	0.0003 (11)	−0.0013 (12)
C10	0.0201 (15)	0.0284 (16)	0.0289 (16)	−0.0034 (12)	0.0030 (12)	−0.0039 (12)
C11	0.0292 (17)	0.0220 (16)	0.0273 (16)	−0.0047 (12)	0.0056 (13)	0.0031 (12)
C12	0.0270 (16)	0.0233 (15)	0.0227 (15)	−0.0004 (12)	0.0027 (12)	0.0011 (11)
C13	0.0203 (14)	0.0182 (14)	0.0226 (14)	0.0009 (11)	0.0043 (11)	−0.0021 (11)
C14	0.0265 (15)	0.0178 (15)	0.0227 (15)	0.0003 (12)	0.0043 (12)	0.0005 (11)
C15	0.0220 (14)	0.0176 (14)	0.0194 (14)	−0.0005 (11)	0.0053 (11)	−0.0025 (11)
C16	0.0255 (15)	0.0203 (15)	0.0218 (14)	−0.0005 (12)	0.0024 (12)	0.0021 (11)
C17	0.0261 (15)	0.0226 (15)	0.0223 (14)	0.0021 (12)	−0.0004 (12)	−0.0024 (11)
C18	0.0186 (14)	0.0208 (15)	0.0243 (14)	0.0018 (11)	0.0011 (11)	−0.0065 (11)
C19	0.0221 (15)	0.0168 (14)	0.0237 (14)	−0.0012 (11)	0.0076 (12)	−0.0001 (11)
C20	0.0224 (15)	0.0187 (14)	0.0187 (14)	0.0067 (11)	0.0044 (11)	−0.0042 (11)
C21	0.0301 (17)	0.043 (2)	0.046 (2)	−0.0013 (14)	0.0111 (15)	0.0236 (15)
C22	0.0232 (15)	0.0272 (15)	0.0274 (15)	−0.0058 (12)	0.0046 (12)	−0.0019 (12)

Geometric parameters (Å, °)

O1—C1	1.356 (3)	C9—C10	1.390 (4)
O1—H1O1	0.87 (4)	C9—H9A	0.9300
O2—C3	1.364 (3)	C10—C11	1.377 (4)
O2—C21	1.432 (3)	C10—H10A	0.9300
O3—C20	1.309 (3)	C11—C12	1.389 (4)
O3—H1O3	1.028 (10)	C11—H11A	0.9300
O4—C18	1.358 (3)	C12—C13	1.398 (4)
O4—C22	1.433 (3)	C12—H12A	0.9300
N1—C7	1.285 (3)	C14—C15	1.417 (4)
N1—C8	1.426 (3)	C14—H14A	0.9300
N2—C14	1.306 (3)	C15—C16	1.407 (4)
N2—C13	1.414 (3)	C15—C20	1.441 (4)
C1—C2	1.382 (4)	C16—C17	1.359 (4)
C1—C6	1.412 (4)	C16—H16A	0.9300
C2—C3	1.385 (4)	C17—C18	1.420 (4)
C2—H2A	0.9300	C17—H17A	0.9300
C3—C4	1.393 (4)	C18—C19	1.374 (4)
C4—C5	1.371 (4)	C19—C20	1.403 (4)
C4—H4A	0.9300	C19—H19A	0.9300
C5—C6	1.406 (4)	C21—H21A	0.9600
C5—H5A	0.9300	C21—H21B	0.9600
C6—C7	1.444 (4)	C21—H21C	0.9600
C7—H7A	0.9300	C22—H22A	0.9600
C8—C9	1.391 (4)	C22—H22B	0.9600
C8—C13	1.401 (4)	C22—H22C	0.9600
C1—O1—H1O1	107 (2)	C11—C12—C13	119.9 (3)
C3—O2—C21	117.2 (2)	C11—C12—H12A	120.0
C20—O3—H1O3	106.5 (17)	C13—C12—H12A	120.0
C18—O4—C22	117.4 (2)	C12—C13—C8	119.0 (2)

C7—N1—C8	119.0 (2)	C12—C13—N2	123.8 (2)
C14—N2—C13	125.4 (2)	C8—C13—N2	117.2 (2)
O1—C1—C2	117.9 (2)	N2—C14—C15	121.6 (2)
O1—C1—C6	121.2 (2)	N2—C14—H14A	119.2
C2—C1—C6	120.9 (2)	C15—C14—H14A	119.2
C1—C2—C3	119.6 (2)	C16—C15—C14	120.8 (2)
C1—C2—H2A	120.2	C16—C15—C20	118.9 (2)
C3—C2—H2A	120.2	C14—C15—C20	120.3 (2)
O2—C3—C2	124.1 (2)	C17—C16—C15	121.9 (2)
O2—C3—C4	115.0 (2)	C17—C16—H16A	119.1
C2—C3—C4	120.8 (2)	C15—C16—H16A	119.1
C5—C4—C3	119.3 (2)	C16—C17—C18	119.1 (3)
C5—C4—H4A	120.3	C16—C17—H17A	120.4
C3—C4—H4A	120.3	C18—C17—H17A	120.4
C4—C5—C6	121.6 (3)	O4—C18—C19	124.6 (2)
C4—C5—H5A	119.2	O4—C18—C17	114.6 (2)
C6—C5—H5A	119.2	C19—C18—C17	120.8 (2)
C5—C6—C1	117.7 (2)	C18—C19—C20	121.0 (2)
C5—C6—C7	120.0 (2)	C18—C19—H19A	119.5
C1—C6—C7	122.3 (2)	C20—C19—H19A	119.5
N1—C7—C6	121.2 (2)	O3—C20—C19	120.4 (2)
N1—C7—H7A	119.4	O3—C20—C15	121.4 (2)
C6—C7—H7A	119.4	C19—C20—C15	118.2 (2)
C9—C8—C13	120.3 (2)	O2—C21—H21A	109.5
C9—C8—N1	122.0 (2)	O2—C21—H21B	109.5
C13—C8—N1	117.6 (2)	H21A—C21—H21B	109.5
C10—C9—C8	120.0 (3)	O2—C21—H21C	109.5
C10—C9—H9A	120.0	H21A—C21—H21C	109.5
C8—C9—H9A	120.0	H21B—C21—H21C	109.5
C11—C10—C9	119.9 (3)	O4—C22—H22A	109.5
C11—C10—H10A	120.1	O4—C22—H22B	109.5
C9—C10—H10A	120.1	H22A—C22—H22B	109.5
C10—C11—C12	120.8 (3)	O4—C22—H22C	109.5
C10—C11—H11A	119.6	H22A—C22—H22C	109.5
C12—C11—H11A	119.6	H22B—C22—H22C	109.5
O1—C1—C2—C3	−179.3 (2)	C11—C12—C13—N2	−179.0 (2)
C6—C1—C2—C3	1.8 (4)	C9—C8—C13—C12	−0.3 (4)
C21—O2—C3—C2	5.5 (4)	N1—C8—C13—C12	−176.7 (2)
C21—O2—C3—C4	−173.5 (3)	C9—C8—C13—N2	−179.6 (2)
C1—C2—C3—O2	−178.5 (2)	N1—C8—C13—N2	4.0 (3)
C1—C2—C3—C4	0.5 (4)	C14—N2—C13—C12	−2.1 (4)
O2—C3—C4—C5	177.3 (2)	C14—N2—C13—C8	177.1 (2)
C2—C3—C4—C5	−1.8 (4)	C13—N2—C14—C15	178.2 (2)
C3—C4—C5—C6	0.8 (4)	N2—C14—C15—C16	−177.7 (2)
C4—C5—C6—C1	1.4 (4)	N2—C14—C15—C20	1.9 (4)
C4—C5—C6—C7	179.4 (3)	C14—C15—C16—C17	179.3 (2)
O1—C1—C6—C5	178.4 (2)	C20—C15—C16—C17	−0.2 (4)
C2—C1—C6—C5	−2.7 (4)	C15—C16—C17—C18	1.3 (4)
O1—C1—C6—C7	0.5 (4)	C22—O4—C18—C19	−5.8 (4)

C2—C1—C6—C7	179.3 (2)	C22—O4—C18—C17	174.5 (2)
C8—N1—C7—C6	−178.8 (2)	C16—C17—C18—O4	178.8 (2)
C5—C6—C7—N1	−172.6 (2)	C16—C17—C18—C19	−0.9 (4)
C1—C6—C7—N1	5.3 (4)	O4—C18—C19—C20	179.6 (2)
C7—N1—C8—C9	52.6 (3)	C17—C18—C19—C20	−0.7 (4)
C7—N1—C8—C13	−131.1 (3)	C18—C19—C20—O3	−178.7 (2)
C13—C8—C9—C10	−0.8 (4)	C18—C19—C20—C15	1.8 (4)
N1—C8—C9—C10	175.4 (2)	C16—C15—C20—O3	179.2 (2)
C8—C9—C10—C11	0.4 (4)	C14—C15—C20—O3	−0.4 (4)
C9—C10—C11—C12	1.0 (4)	C16—C15—C20—C19	−1.3 (3)
C10—C11—C12—C13	−2.1 (4)	C14—C15—C20—C19	179.1 (2)
C11—C12—C13—C8	1.8 (4)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1O1···N1	0.87 (3)	1.83 (4)	2.615 (3)	149 (3)
O3—H1O3···N2	1.03 (2)	1.61 (2)	2.555 (3)	150 (2)
C7—H7A···O3^{i}	0.93	2.44	3.283 (3)	150
C10—H10A···O2^{ii}	0.93	2.57	3.362 (3)	143
C12—H12A···Cg1^{iii}	0.93	2.80	3.614 (3)	147
C21—H21A···Cg2^{iv}	0.96	2.56	3.412 (3)	149
C22—H22A···Cg1^{v}	0.96	2.68	3.396 (3)	132

Symmetry codes: (i) *x*−1, *y*, *z*; (ii) −*x*−1, *y*−1/2, −*z*+3/2; (iii) *x*, −*y*−1/2, *z*−1/2; (iv) −*x*, *y*+1/2, −*z*+3/2; (v) −*x*+1, −*y*+1, −*z*+2.

Fig. 1

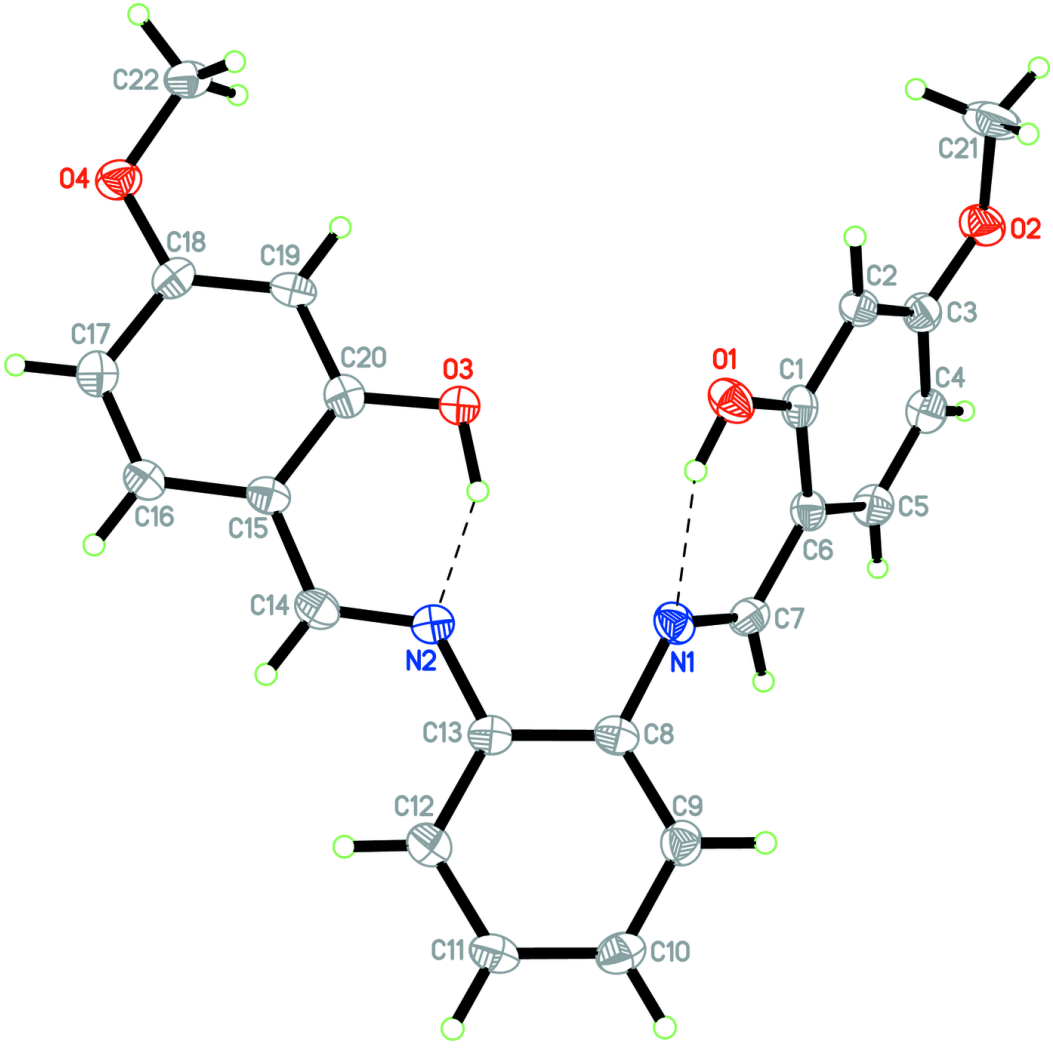
C22
O4
C18
C19
C17
C20
O3
C16
C15
C14
N2
C13
C12
C11
C10
C9
C8
N1
C7
C6
C5
C4
C3
C2
O2
C21
O1
C1

Fig. 2