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2,2′-[(Propane-1,3-diyldinitrilo)bis(phenylmethylidyne)]diphenol

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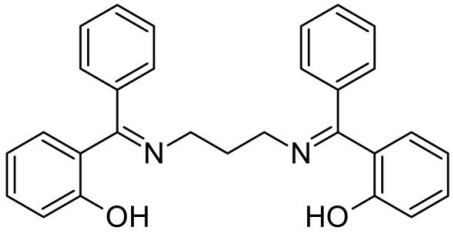
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.055; wR factor = 0.173; data-to-parameter ratio = 19.7.

In the title molecule, $C_{29}H_{26}N_2O_2$, there are two strong intramolecular O—H···N hydrogen bonds involving the hydroxy and imine groups, forming $S(6)$ ring motifs. The dihedral angles between adjacent phenyl rings and phenol-containing planes are 85.27 (19) and 91.38 (18)°. In the crystal structure, weak intermolecular C—H···O hydrogen bonds connect molecules into a two-dimensional network.

Related literature

The title compound forms part of the group of Schiff bases with a similar method of synthesis as described in Schilf *et al.* (2007). The intermolecular hydrogen bonds O—H···N between the hydroxy and imine are common to this type of compound as shown with the series of compounds reported by Fernández *et al.* (2001); Kabak (2003); Wojciechowski *et al.* (2001); Dey *et al.* (2001); Koşar, *et al.* (2004); Lu, *et al.* (2008); Qiu & Zhao (2008); Montazerozohori *et al.* (2009); Corden *et al.* (1996). For a decription of hydrogen-bond motifs, see: Bernstein *et al.* (1995).



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Experimental

Crystal data

$C_{29}H_{26}N_2O_2$
M_r = 434.52
Monoclinic, $P2_1/c$
a = 18.226 (2) Å
b = 8.2303 (9) Å
c = 18.642 (2) Å
β = 119.086 (5)°
V = 2443.7 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.07 mm^{-1}
T = 293 K
0.7 × 0.5 × 0.28 mm

Data collection

Bruker SMART 1K CCD area-detector diffractometer
21350 measured reflections
5896 independent reflections
3749 reflections with $I > 2\sigma(I)$
R_{int} = 0.071

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.173
S = 1.03
5896 reflections
300 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1A···N1	0.82	1.80	2.5344 (17)	148
O2—H2A···N2	0.82	1.81	2.5431 (18)	148
C17—H17···O2^{i}	0.93	2.56	3.481 (2)	168
C18—H18···O1^{ii}	0.93	2.47	3.395 (3)	174
C21—H21···O2^{iii}	0.93	2.56	3.492 (2)	175

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

Data collection: *SMART-NT* (Bruker, 1998); cell refinement: *SAINT-Plus* (Bruker, 1999); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON*.

The University of the Witwatersrand and the National Research Foundation (GUN 2069064) are thanked for providing the infrastructure and for the award of a research grant required to carry out this work.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH5012).

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supplementary materials

Acta Cryst. (2010). E**66**, o1002-o1003 [**doi:10.1107/S1600536810011189**]

2,2'-[(Propane-1,3-diyldinitrilo)bis(phenylmethylidyne)]diphenol

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Comment

The molecular structure of the title compound is shown in Fig. 1. There are two strong intramolecular O—H..O hydrogen bonds involving the hydroxyl and imine groups forming S(6) ring motifs (Bernstein *et al.*, 1995). These types of hydrogen bonds are common to some reported molecular structures (Schilf *et al.*, 2007; Fernández *et al.*, 2001; Kabak, 2003; Wojciechowski *et al.*, 2001; Dey *et al.*, 2001; Koşar, *et al.*, 2004; Lu, *et al.*, 2008; Qiu & Zhao, 2008; Montazerozohori *et al.,* 2009; Corden *et al.*, 1996). In the crystal structure, weak intermolecular C—H···O hydrogen bond connect molecules to form a two-dimensional network.

Experimental

A mixture of 1.0 mmol (2.00 g) of 2-hydroxybenzophenone, 0.5 mmole (0.42 cm^3) of 1,3-propanediamine and 2 drops of glacial acetic acid in 40 ml of methanol was refluxed for 8 h. The excess of solvent (ca. 30 ml) was then evaporated. After cooling to 277 K a yellow solid was produced. The polycrystalline product was collected by filtration, washed with methanol and dried. A yield of 52% was obtained. Recrystalization from an ethanol solution yielded single crystals suitable for x-ray diffraction. Elemental analysis *C% 79.67 H% 6.26 N% 6.11%.*

Refinement

All H atoms were refined using a riding model, with C—H = 0.93-0.97 Å, O—H = 0.82 Å, and *U*iso(H) = 1.2*U*eq(C) or 1.5*U*eq(O).

Figures

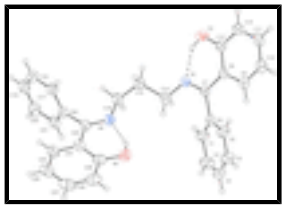


Fig. 1. The molecular structure of the title compound with displacement ellipsoids drawn at the 30% probability level. Hydrogen bonds are shown as dashed lines.

2,2'-[(Propane-1,3-diyldinitrilo)bis(phenylmethylidyne)]diphenol

Crystal data

$C_{29}H_{26}N_2O_2$	$F(000) = 920$
$M_r = 434.52$	$D_x = 1.181$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Hall symbol: -P 2ybc	Cell parameters from 21350 reflections
a = 18.226 (2) Å	θ = 2.1–23.0°
b = 8.2303 (9) Å	μ = 0.07 mm^{-1}
c = 18.642 (2) Å	T = 293 K
β = 119.086 (5)°	Block, yellow
V = 2443.7 (5) Å^3	0.7 × 0.5 × 0.28 mm
Z = 4	

Data collection

Bruker SMART 1K CCD area-detector diffractometer	R_{int} = 0.071
φ and ω scans	θ_{max} = 28°, θ_{min} = 1.3°
21350 measured reflections	h = −19→24
5896 independent reflections	k = −10→10
3749 reflections with $I > 2\sigma(I)$	l = −24→20

Refinement

Refinement on F^2	0 restraints
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.055	$w = 1/[\sigma^2(F_o^2) + (0.0897P)^2 + 0.2258P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.173	$(\Delta/\sigma)_{max}$ = 0.002
S = 1.03	$\Delta\rho_{max}$ = 0.23 e Å^{-3}
5896 reflections	$\Delta\rho_{min}$ = −0.36 e Å^{-3}
300 parameters	

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

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

	x	y	z	U_{iso}*/U_{eq}
C1	0.17087 (13)	0.1655 (3)	0.08228 (11)	0.0718 (5)
H1	0.1926	0.2672	0.0813	0.086*
C2	0.15625 (16)	0.0517 (3)	0.02117 (14)	0.0940 (7)
H2	0.1689	0.0776	−0.0201	0.113*
C3	0.12367 (14)	−0.0961 (3)	0.02162 (16)	0.0947 (8)
H3	0.1142	−0.1708	−0.0194	0.114*
C4	0.10480 (16)	−0.1362 (3)	0.08146 (16)	0.0960 (7)
H4	0.0823	−0.2377	0.0812	0.115*
C5	0.11925 (13)	−0.0247 (3)	0.14328 (13)	0.0759 (5)

H5	0.1062	−0.0519	0.1842	0.091*
C6	0.15300 (9)	0.12641 (19)	0.14400 (9)	0.0501 (4)
C7	0.17057 (8)	0.24201 (18)	0.21320 (9)	0.0457 (3)
C8	0.10782 (9)	0.36732 (18)	0.20194 (9)	0.0476 (3)
C9	0.03699 (10)	0.3944 (2)	0.12497 (11)	0.0612 (4)
H9	0.0291	0.3308	0.0805	0.073*
C10	−0.02150 (12)	0.5138 (3)	0.11365 (13)	0.0775 (6)
H10	−0.0675	0.5312	0.062	0.093*
C11	−0.01072 (13)	0.6066 (3)	0.17994 (16)	0.0826 (6)
H11	−0.05	0.6861	0.1726	0.099*
C12	0.05729 (13)	0.5829 (2)	0.25660 (14)	0.0735 (5)
H12	0.0632	0.6461	0.3004	0.088*
C13	0.11810 (10)	0.4642 (2)	0.26941 (10)	0.0548 (4)
C14	0.30624 (10)	0.1168 (2)	0.29798 (11)	0.0637 (4)
H14A	0.3103	0.1037	0.2483	0.076*
H14B	0.2935	0.0117	0.3128	0.076*
C15	0.38907 (10)	0.1788 (2)	0.36662 (10)	0.0590 (4)
H15A	0.385	0.1869	0.4165	0.071*
H15B	0.3992	0.287	0.3528	0.071*
C16	0.46364 (10)	0.0702 (2)	0.38294 (10)	0.0606 (4)
H16A	0.5125	0.1034	0.4336	0.073*
H16B	0.4508	−0.0416	0.3891	0.073*
C17	0.66693 (10)	0.2305 (2)	0.45511 (10)	0.0602 (4)
H17	0.6442	0.3306	0.4316	0.072*
C18	0.73422 (12)	0.2233 (3)	0.53470 (12)	0.0729 (5)
H18	0.756	0.3185	0.5644	0.087*
C19	0.76854 (12)	0.0763 (3)	0.56945 (12)	0.0743 (5)
H19	0.813	0.0721	0.6229	0.089*
C20	0.73734 (12)	−0.0646 (3)	0.52550 (13)	0.0747 (5)
H20	0.7618	−0.1637	0.5489	0.09*
C21	0.66949 (11)	−0.0604 (2)	0.44627 (11)	0.0608 (4)
H21	0.6481	−0.1564	0.4172	0.073*
C22	0.63373 (9)	0.08832 (18)	0.41069 (9)	0.0469 (3)
C23	0.55780 (9)	0.09263 (18)	0.32620 (9)	0.0496 (4)
C24	0.57020 (11)	0.10567 (19)	0.25341 (10)	0.0539 (4)
C25	0.65069 (12)	0.1279 (2)	0.26229 (12)	0.0676 (5)
H25	0.6968	0.134	0.3147	0.081*
C26	0.66269 (15)	0.1409 (3)	0.19441 (15)	0.0808 (6)
H26	0.7163	0.156	0.2012	0.097*
C27	0.59361 (18)	0.1312 (3)	0.11627 (15)	0.0861 (7)
H27	0.6013	0.1387	0.0706	0.103*
C28	0.51399 (16)	0.1106 (2)	0.10547 (12)	0.0769 (6)
H28	0.4686	0.1045	0.0527	0.092*
C29	0.50056 (12)	0.09859 (19)	0.17301 (11)	0.0597 (4)
N1	0.23864 (8)	0.23289 (17)	0.28316 (8)	0.0562 (3)
N2	0.48206 (8)	0.08218 (17)	0.31467 (8)	0.0564 (3)
O1	0.18408 (8)	0.44387 (17)	0.34460 (7)	0.0709 (4)
H1A	0.2167	0.3781	0.3424	0.106*
O2	0.42130 (8)	0.08050 (17)	0.15964 (7)	0.0715 (4)

H2A	0.4218	0.074	0.2038	0.107*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0820 (13)	0.0800 (12)	0.0680 (11)	−0.0146 (10)	0.0478 (10)	−0.0153 (9)
C2	0.1009 (17)	0.125 (2)	0.0795 (14)	−0.0200 (15)	0.0625 (14)	−0.0331 (13)
C3	0.0776 (14)	0.1138 (19)	0.1001 (16)	−0.0262 (13)	0.0490 (13)	−0.0609 (14)
C4	0.0966 (17)	0.0856 (15)	0.1172 (18)	−0.0384 (13)	0.0610 (16)	−0.0465 (14)
C5	0.0807 (13)	0.0769 (12)	0.0816 (13)	−0.0279 (10)	0.0484 (11)	−0.0252 (10)
C6	0.0390 (7)	0.0596 (9)	0.0508 (8)	−0.0030 (6)	0.0212 (6)	−0.0107 (7)
C7	0.0393 (7)	0.0540 (8)	0.0465 (7)	−0.0056 (6)	0.0229 (6)	−0.0073 (6)
C8	0.0400 (7)	0.0531 (8)	0.0529 (8)	−0.0062 (6)	0.0250 (7)	−0.0070 (6)
C9	0.0456 (9)	0.0714 (11)	0.0615 (10)	−0.0002 (7)	0.0220 (8)	−0.0086 (8)
C10	0.0513 (10)	0.0855 (13)	0.0823 (13)	0.0124 (9)	0.0221 (9)	−0.0007 (11)
C11	0.0607 (12)	0.0732 (12)	0.1165 (18)	0.0144 (9)	0.0451 (13)	−0.0065 (12)
C12	0.0679 (12)	0.0709 (12)	0.0926 (14)	0.0000 (9)	0.0475 (11)	−0.0229 (10)
C13	0.0520 (9)	0.0573 (9)	0.0625 (10)	−0.0083 (7)	0.0338 (8)	−0.0127 (7)
C14	0.0450 (9)	0.0724 (11)	0.0627 (10)	0.0065 (7)	0.0175 (8)	−0.0136 (8)
C15	0.0442 (8)	0.0750 (11)	0.0546 (9)	−0.0015 (7)	0.0217 (7)	−0.0083 (8)
C16	0.0435 (8)	0.0848 (12)	0.0528 (9)	0.0052 (8)	0.0229 (7)	0.0092 (8)
C17	0.0553 (9)	0.0568 (9)	0.0662 (10)	−0.0005 (7)	0.0277 (8)	−0.0048 (8)
C18	0.0569 (10)	0.0913 (14)	0.0704 (12)	−0.0188 (10)	0.0310 (9)	−0.0281 (10)
C19	0.0501 (10)	0.1127 (17)	0.0548 (10)	0.0029 (10)	0.0213 (8)	0.0014 (10)
C20	0.0621 (11)	0.0852 (14)	0.0726 (12)	0.0204 (10)	0.0294 (10)	0.0230 (11)
C21	0.0566 (10)	0.0567 (9)	0.0669 (10)	0.0052 (7)	0.0282 (9)	0.0009 (8)
C22	0.0402 (7)	0.0523 (8)	0.0505 (8)	0.0024 (6)	0.0237 (7)	−0.0007 (6)
C23	0.0455 (8)	0.0508 (8)	0.0518 (8)	0.0035 (6)	0.0230 (7)	−0.0005 (6)
C24	0.0605 (9)	0.0511 (8)	0.0554 (9)	0.0042 (7)	0.0324 (8)	−0.0011 (7)
C25	0.0690 (11)	0.0714 (11)	0.0764 (12)	0.0021 (9)	0.0465 (10)	−0.0025 (9)
C26	0.0994 (16)	0.0749 (13)	0.1028 (16)	0.0019 (11)	0.0763 (15)	−0.0001 (11)
C27	0.136 (2)	0.0732 (13)	0.0831 (15)	0.0020 (13)	0.0797 (16)	0.0013 (11)
C28	0.1119 (17)	0.0633 (11)	0.0601 (11)	0.0001 (11)	0.0456 (12)	−0.0017 (8)
C29	0.0754 (12)	0.0501 (9)	0.0562 (9)	0.0028 (8)	0.0340 (9)	−0.0002 (7)
N1	0.0429 (7)	0.0685 (9)	0.0517 (7)	0.0042 (6)	0.0187 (6)	−0.0111 (6)
N2	0.0442 (7)	0.0732 (9)	0.0494 (7)	0.0036 (6)	0.0209 (6)	0.0030 (6)
O1	0.0677 (8)	0.0854 (9)	0.0572 (7)	0.0013 (6)	0.0285 (6)	−0.0219 (6)
O2	0.0667 (8)	0.0858 (9)	0.0505 (6)	−0.0029 (6)	0.0193 (6)	−0.0008 (6)

Geometric parameters (Å, °)

C1—C6	1.378 (2)	C15—H15B	0.97
C1—C2	1.396 (3)	C16—N2	1.469 (2)
C1—H1	0.93	C16—H16A	0.97
C2—C3	1.356 (3)	C16—H16B	0.97
C2—H2	0.93	C17—C22	1.391 (2)
C3—C4	1.358 (3)	C17—C18	1.393 (3)
C3—H3	0.93	C17—H17	0.93
C4—C5	1.394 (3)	C18—C19	1.371 (3)

C4—H4	0.93	C18—H18	0.93
C5—C6	1.385 (2)	C19—C20	1.374 (3)
C5—H5	0.93	C19—H19	0.93
C6—C7	1.507 (2)	C20—C21	1.392 (3)
C7—N1	1.2934 (19)	C20—H20	0.93
C7—C8	1.477 (2)	C21—C22	1.394 (2)
C8—C9	1.405 (2)	C21—H21	0.93
C8—C13	1.422 (2)	C22—C23	1.509 (2)
C9—C10	1.389 (3)	C23—N2	1.293 (2)
C9—H9	0.93	C23—C24	1.484 (2)
C10—C11	1.383 (3)	C24—C25	1.406 (2)
C10—H10	0.93	C24—C29	1.418 (2)
C11—C12	1.376 (3)	C25—C26	1.389 (3)
C11—H11	0.93	C25—H25	0.93
C12—C13	1.408 (2)	C26—C27	1.389 (3)
C12—H12	0.93	C26—H26	0.93
C13—O1	1.342 (2)	C27—C28	1.375 (3)
C14—N1	1.475 (2)	C27—H27	0.93
C14—C15	1.516 (2)	C28—C29	1.398 (3)
C14—H14A	0.97	C28—H28	0.93
C14—H14B	0.97	C29—O2	1.349 (2)
C15—C16	1.528 (2)	O1—H1A	0.82
C15—H15A	0.97	O2—H2A	0.82
C6—C1—C2	119.74 (19)	H15A—C15—H15B	107.7
C6—C1—H1	120.1	N2—C16—C15	110.13 (13)
C2—C1—H1	120.1	N2—C16—H16A	109.6
C3—C2—C1	120.5 (2)	C15—C16—H16A	109.6
C3—C2—H2	119.8	N2—C16—H16B	109.6
C1—C2—H2	119.8	C15—C16—H16B	109.6
C2—C3—C4	120.63 (19)	H16A—C16—H16B	108.1
C2—C3—H3	119.7	C22—C17—C18	120.06 (16)
C4—C3—H3	119.7	C22—C17—H17	120
C3—C4—C5	119.9 (2)	C18—C17—H17	120
C3—C4—H4	120.1	C19—C18—C17	120.31 (18)
C5—C4—H4	120.1	C19—C18—H18	119.8
C6—C5—C4	120.23 (19)	C17—C18—H18	119.8
C6—C5—H5	119.9	C18—C19—C20	120.11 (17)
C4—C5—H5	119.9	C18—C19—H19	119.9
C1—C6—C5	119.07 (16)	C20—C19—H19	119.9
C1—C6—C7	121.98 (15)	C19—C20—C21	120.55 (17)
C5—C6—C7	118.94 (15)	C19—C20—H20	119.7
N1—C7—C8	118.72 (13)	C21—C20—H20	119.7
N1—C7—C6	121.82 (13)	C20—C21—C22	119.74 (16)
C8—C7—C6	119.45 (12)	C20—C21—H21	120.1
C9—C8—C13	118.36 (14)	C22—C21—H21	120.1
C9—C8—C7	121.28 (13)	C17—C22—C21	119.22 (15)
C13—C8—C7	120.37 (13)	C17—C22—C23	120.95 (13)
C10—C9—C8	121.58 (17)	C21—C22—C23	119.78 (13)
C10—C9—H9	119.2	N2—C23—C24	118.54 (14)

C8—C9—H9	119.2	N2—C23—C22	122.36 (14)
C11—C10—C9	119.33 (19)	C24—C23—C22	119.09 (13)
C11—C10—H10	120.3	C25—C24—C29	118.44 (16)
C9—C10—H10	120.3	C25—C24—C23	121.04 (15)
C12—C11—C10	120.99 (17)	C29—C24—C23	120.51 (15)
C12—C11—H11	119.5	C26—C25—C24	121.34 (19)
C10—C11—H11	119.5	C26—C25—H25	119.3
C11—C12—C13	120.75 (17)	C24—C25—H25	119.3
C11—C12—H12	119.6	C27—C26—C25	119.15 (19)
C13—C12—H12	119.6	C27—C26—H26	120.4
O1—C13—C12	119.70 (15)	C25—C26—H26	120.4
O1—C13—C8	121.33 (14)	C28—C27—C26	120.96 (18)
C12—C13—C8	118.98 (16)	C28—C27—H27	119.5
N1—C14—C15	109.80 (14)	C26—C27—H27	119.5
N1—C14—H14A	109.7	C27—C28—C29	120.7 (2)
C15—C14—H14A	109.7	C27—C28—H28	119.6
N1—C14—H14B	109.7	C29—C28—H28	119.6
C15—C14—H14B	109.7	O2—C29—C28	118.80 (17)
H14A—C14—H14B	108.2	O2—C29—C24	121.83 (15)
C14—C15—C16	113.32 (14)	C28—C29—C24	119.37 (18)
C14—C15—H15A	108.9	C7—N1—C14	122.06 (13)
C16—C15—H15A	108.9	C23—N2—C16	122.40 (13)
C14—C15—H15B	108.9	C13—O1—H1A	109.5
C16—C15—H15B	108.9	C29—O2—H2A	109.5
C6—C1—C2—C3	0.8 (4)	C18—C19—C20—C21	−1.6 (3)
C1—C2—C3—C4	−0.1 (4)	C19—C20—C21—C22	1.0 (3)
C2—C3—C4—C5	−0.2 (4)	C18—C17—C22—C21	−1.1 (2)
C3—C4—C5—C6	−0.2 (4)	C18—C17—C22—C23	176.55 (14)
C2—C1—C6—C5	−1.2 (3)	C20—C21—C22—C17	0.3 (2)
C2—C1—C6—C7	177.65 (19)	C20—C21—C22—C23	−177.36 (15)
C4—C5—C6—C1	0.9 (3)	C17—C22—C23—N2	−90.01 (19)
C4—C5—C6—C7	−177.97 (19)	C21—C22—C23—N2	87.61 (19)
C1—C6—C7—N1	−96.1 (2)	C17—C22—C23—C24	91.38 (18)
C5—C6—C7—N1	82.8 (2)	C21—C22—C23—C24	−91.00 (18)
C1—C6—C7—C8	85.27 (19)	N2—C23—C24—C25	175.86 (15)
C5—C6—C7—C8	−95.88 (19)	C22—C23—C24—C25	−5.5 (2)
N1—C7—C8—C9	173.25 (15)	N2—C23—C24—C29	−3.1 (2)
C6—C7—C8—C9	−8.1 (2)	C22—C23—C24—C29	175.57 (13)
N1—C7—C8—C13	−6.6 (2)	C29—C24—C25—C26	−0.7 (3)
C6—C7—C8—C13	172.08 (13)	C23—C24—C25—C26	−179.70 (16)
C13—C8—C9—C10	1.0 (3)	C24—C25—C26—C27	−0.2 (3)
C7—C8—C9—C10	−178.90 (17)	C25—C26—C27—C28	0.7 (3)
C8—C9—C10—C11	−1.2 (3)	C26—C27—C28—C29	−0.1 (3)
C9—C10—C11—C12	0.5 (3)	C27—C28—C29—O2	179.16 (17)
C10—C11—C12—C13	0.4 (3)	C27—C28—C29—C24	−0.9 (3)
C11—C12—C13—O1	179.67 (18)	C25—C24—C29—O2	−178.77 (16)
C11—C12—C13—C8	−0.6 (3)	C23—C24—C29—O2	0.2 (2)
C9—C8—C13—O1	179.63 (15)	C25—C24—C29—C28	1.2 (2)
C7—C8—C13—O1	−0.5 (2)	C23—C24—C29—C28	−179.77 (15)

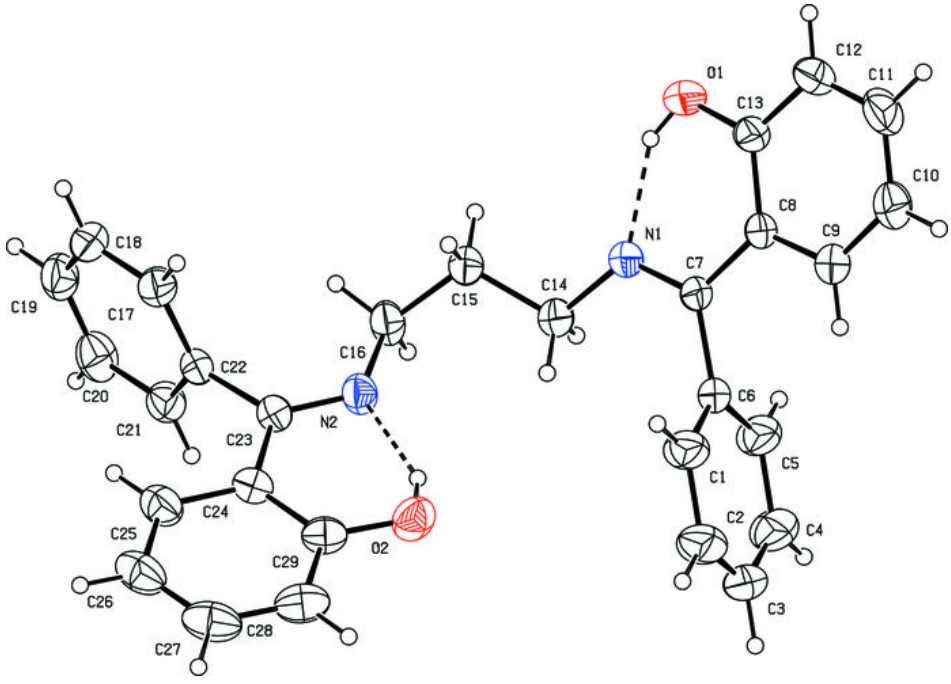
C9—C8—C13—C12	−0.1 (2)	C8—C7—N1—C14	−176.84 (14)
C7—C8—C13—C12	179.80 (15)	C6—C7—N1—C14	4.5 (2)
N1—C14—C15—C16	−176.82 (14)	C15—C14—N1—C7	155.47 (15)
C14—C15—C16—N2	70.2 (2)	C24—C23—N2—C16	−179.47 (14)
C22—C17—C18—C19	0.5 (3)	C22—C23—N2—C16	1.9 (2)
C17—C18—C19—C20	0.8 (3)	C15—C16—N2—C23	137.49 (16)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1A···N1	0.82	1.80	2.5344 (17)	148
O2—H2A···N2	0.82	1.81	2.5431 (18)	148
C17—H17···O2^{i}	0.93	2.56	3.481 (2)	168
C18—H18···O1^{ii}	0.93	2.47	3.395 (3)	174
C21—H21···O2^{iii}	0.93	2.56	3.492 (2)	175

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

Fig. 1


C12
O1
C11
C13
C10
C8
C9
N1
C7
C18
C14
C15
C19
C17
C16
C22
C6
C20
N2
C21
C23
C5
C1
C24
C2
C4
C25
O2
C29
C26
C3
C28
C27