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# *N*,*N*′-Bis[(2-hydroxyphenyl)(phenyl)methylidene]propane-1,2-diamine

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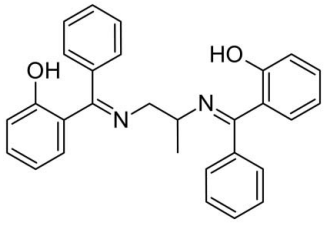
Key indicators: single-crystal X-ray study; $T$ = 296 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.034; $wR$ factor = 0.087; data-to-parameter ratio = 10.0.

In the the title compound, $C_{29}H_{26}N_2O_2$, two strong intramolecular O—H···N hydrogen bonds involving the hydroxy and imine groups generate $S$(6) ring motifs. The dihedral angles between the pairs of terminal benzene rings are 89.8 (2) and 87.8 (2)°.

## Related literature

For related compounds and further synthetic details, see: Schilf *et al.* (2007). For intramolecular hydrogen bonds in this type of compound, see: Fernández-G *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); Black *et al.* (2010); Dey *et al.* (2001).




## Experimental

### *Crystal data*

$C_{29}H_{26}N_2O_2$
$M_r$ = 434.52
Monoclinic, $C2$
$a$ = 18.1766 (8) Å
$b$ = 7.9808 (4) Å
$c$ = 16.0347 (8) Å
$\beta$ = 92.703 (2)°
$V$ = 2323.47 (19) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.08 mm$^{-1}$
$T$ = 296 K
0.62 × 0.38 × 0.24 mm

### *Data collection*

Bruker APEXII CCD diffractometer
Absorption correction: integration (*XPREP*; Bruker, 1999)
$T_{min}$ = 0.918, $T_{max}$ = 1.000
22291 measured reflections
3001 independent reflections
2724 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.026

### *Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.087
$S$ = 1.05
3001 reflections
301 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.20 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.18 e Å$^{-3}$

**Table 1**
Selected torsion angles (°).

| | | | |
|---|---|---|---|
| C1—C6—C7—C8 | 89.8 (2) | C17—C22—C23—C24 | 87.8 (2) |

**Table 2**
Hydrogen-bond geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O1—H1*A*···N1 | 0.82 | 1.84 | 2.573 (2) | 147 |
| O2—H2*A*···N2 | 0.82 | 1.83 | 2.553 (2) | 147 |

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT-NT* (Bruker, 2005); data reduction: *SAINT-NT*; program(s) used to solve structure: *SHELXTL* (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: HB5392).

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# supplementary materials

*Acta Cryst.* (2010). E**66**, o1256-o1257 [ **doi:10.1107/S1600536810015291** ]

# *N*,*N*'-Bis[(2-hydroxyphenyl)(phenyl)methylidene]propane-1,2-diamine

**R. S. Black, D. G. Billing, A. Bartyzel and E. M. Cukrowska**

## Comment

The molecular structure of the title compound form two strong intermolecular hydrogen bonds O—H···N involving the hydroxyl and the imine groups, forming S(6) ring motifs which are common to this type of compound (Schilf *et al.*, 2007) and (Fernández-G *et al.*, 2001), and also seen in the work completed by (Kabak *et al.*, 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) and (Black *et al.*, 2010). This causes the dihedral angles between the adjacent phenyl rings and phenyl containing plains to be (C1—C6—C7—C8) 89.8 (2)° and (C17—C22—C23—C24) 87.8 (2)° respectively. These dihedral angles are comparable to (Corden *et al.*, 1996) and (Black *et al.*, 2010). The stereogenic centre on the methyl substituted carbon C15 allows the system to pack in the noncentrosymmetric space group *C2*. The remaining weak interactions in the crystals form unexceptional σ-π interactions.

## Experimental

A mixture of 0.01 mol (2.00 g) of 2-hydroxybenzophenone and 0.005 mole (0.42 ml) of 1,2-propanediamine in 40 ml of methanol was refluxed for 7 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 54% was obtained. Recrystalization from an ethanol solution yielded yellow blocks of (I). Elemental analysis: *C% 79.67 H% 5.99 N% 6.03*.

## Refinement

The absolute structure of (I) is indeterminate based on the present refinement. All H atoms were refined using a riding model, with a C—H distance of 0.96, for Ar—H a distance of 0.93 Å and for O—H a distance of 0.82 Å, and *U*iso(H) = 1.2*U*eq(C) and 1.5*U*eq(O). The highest residual peak was 0.742 Å from atom C6 with a ρ = 0.20 e Å$^{-3}$.

## Figures

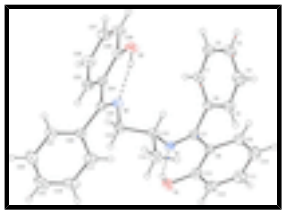


Fig. 1. The molecular structure of (I) drawn at the 30% probability displacement ellipsoids. Hydrogens bonds are shown as dashed lines.

### *N*,*N*'-Bis[(2-hydroxyphenyl)(phenyl)methylidene]propane-1,2-diamine

*Crystal data*

| | |
|---|---|
| $C_{29}H_{26}N_2O_2$ | $F(000) = 920$ |
| $M_r = 434.52$ | $D_x = 1.242$ Mg m$^{-3}$ |
| Monoclinic, *C*2 | Mo *K*α radiation, λ = 0.71073 Å |
| Hall symbol: C 2y | Cell parameters from 9931 reflections |
| $a = 18.1766$ (8) Å | θ = 2.2–28.3° |
| $b = 7.9808$ (4) Å | μ = 0.08 mm$^{-1}$ |
| $c = 16.0347$ (8) Å | $T = 296$ K |
| β = 92.703 (2)° | Block, yellow |
| $V = 2323.47$ (19) Å$^3$ | 0.62 × 0.38 × 0.24 mm |
| $Z = 4$ | |

*Data collection*

| | |
|---|---|
| Bruker APEXII CCD diffractometer | 3001 independent reflections |
| Radiation source: sealed tube | 2724 reflections with $I > 2\sigma(I)$ |
| graphite | $R_{int} = 0.026$ |
| φ and ω scans | $\theta_{max} = 28°$, $\theta_{min} = 1.3°$ |
| Absorption correction: integration (XPREP; Bruker, 1999) | $h = -23\rightarrow24$ |
| $T_{min} = 0.918$, $T_{max} = 1.000$ | $k = -10\rightarrow10$ |
| 22291 measured reflections | $l = -21\rightarrow20$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | 1 restraint |
| Least-squares matrix: full | H-atom parameters constrained |
| $R[F^2 > 2\sigma(F^2)] = 0.034$ | $w = 1/[\sigma^2(F_o^2) + (0.0448P)^2 + 0.6417P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $wR(F^2) = 0.087$ | $(\Delta/\sigma)_{max} = 0.001$ |
| $S = 1.05$ | $\Delta\rho_{max} = 0.20$ e Å$^{-3}$ |
| 3001 reflections | $\Delta\rho_{min} = -0.18$ e Å$^{-3}$ |
| 301 parameters | |

*Special details*

**Experimental**. Numerical integration absorption corrections based on indexed crystal faces were applied using the XPREP routine (Bruker, 1999)

**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 | 0.17117 (10) | 0.8773 (3) | 0.19104 (12) | 0.0380 (4) |
| H1 | 0.1576 | 0.8561 | 0.2453 | 0.046* |
| C2 | 0.23795 (11) | 0.9528 (3) | 0.17780 (14) | 0.0452 (5) |
| H2 | 0.2699 | 0.9792 | 0.2229 | 0.054* |
| C3 | 0.25725 (11) | 0.9890 (3) | 0.09795 (15) | 0.0500 (5) |
| H3 | 0.302 | 1.0411 | 0.0891 | 0.06* |
| C4 | 0.21054 (12) | 0.9484 (3) | 0.03135 (14) | 0.0536 (5) |
| H4 | 0.2237 | 0.974 | −0.0225 | 0.064* |
| C5 | 0.14368 (11) | 0.8693 (3) | 0.04351 (12) | 0.0432 (5) |
| H5 | 0.1124 | 0.8412 | −0.0019 | 0.052* |
| C6 | 0.12418 (9) | 0.8328 (2) | 0.12419 (11) | 0.0318 (4) |
| C7 | 0.05455 (9) | 0.7387 (2) | 0.14143 (10) | 0.0308 (4) |
| C8 | −0.01204 (10) | 0.8365 (2) | 0.15614 (11) | 0.0317 (4) |
| C9 | −0.01477 (11) | 1.0091 (2) | 0.14096 (13) | 0.0398 (4) |
| H9 | 0.0267 | 1.0624 | 0.1219 | 0.048* |
| C10 | −0.07704 (12) | 1.1025 (3) | 0.15342 (13) | 0.0478 (5) |
| H10 | −0.0777 | 1.2167 | 0.142 | 0.057* |
| C11 | −0.13872 (12) | 1.0242 (3) | 0.18322 (14) | 0.0487 (5) |
| H11 | −0.1808 | 1.0867 | 0.1924 | 0.058* |
| C12 | −0.13812 (11) | 0.8549 (3) | 0.19929 (13) | 0.0445 (5) |
| H12 | −0.1796 | 0.8042 | 0.2199 | 0.053* |
| C13 | −0.07625 (10) | 0.7587 (3) | 0.18505 (12) | 0.0372 (4) |
| C14 | 0.09851 (12) | 0.3771 (3) | 0.04854 (12) | 0.0445 (5) |
| H14A | 0.0548 | 0.3114 | 0.0545 | 0.067* |
| H14B | 0.139 | 0.3044 | 0.0374 | 0.067* |
| H14C | 0.0907 | 0.4544 | 0.0031 | 0.067* |
| C15 | 0.11599 (10) | 0.4740 (2) | 0.12901 (11) | 0.0330 (4) |
| H15 | 0.1592 | 0.5453 | 0.1221 | 0.04* |
| C16 | 0.13115 (11) | 0.3541 (2) | 0.20186 (11) | 0.0364 (4) |
| H16A | 0.0869 | 0.2909 | 0.2124 | 0.044* |
| H16B | 0.1695 | 0.2755 | 0.1882 | 0.044* |
| C17 | −0.00368 (11) | 0.3145 (3) | 0.35288 (13) | 0.0447 (5) |
| H17 | −0.0215 | 0.4205 | 0.3389 | 0.054* |
| C18 | −0.05238 (12) | 0.1829 (4) | 0.36563 (14) | 0.0602 (7) |
| H18 | −0.1029 | 0.2012 | 0.3604 | 0.072* |
| C19 | −0.02579 (16) | 0.0266 (4) | 0.38587 (16) | 0.0640 (7) |
| H19 | −0.0585 | −0.0607 | 0.3944 | 0.077* |
| C20 | 0.04851 (16) | −0.0019 (3) | 0.39361 (17) | 0.0639 (7) |
| H20 | 0.066 | −0.1085 | 0.4071 | 0.077* |
| C21 | 0.09762 (13) | 0.1270 (3) | 0.38147 (14) | 0.0477 (5) |
| H21 | 0.148 | 0.1073 | 0.3869 | 0.057* |
| C22 | 0.07149 (10) | 0.2860 (2) | 0.36114 (11) | 0.0331 (4) |
| C23 | 0.12560 (9) | 0.4238 (2) | 0.34679 (11) | 0.0307 (3) |
| C24 | 0.14855 (9) | 0.5331 (2) | 0.41770 (11) | 0.0304 (3) |
| C25 | 0.11331 (10) | 0.5252 (2) | 0.49331 (12) | 0.0368 (4) |

| | | | | |
|---|---|---|---|---|
| H25 | 0.0749 | 0.4495 | 0.4988 | 0.044* |
| C26 | 0.13414 (11) | 0.6270 (3) | 0.56007 (13) | 0.0437 (5) |
| H26 | 0.1102 | 0.6195 | 0.6099 | 0.052* |
| C27 | 0.19109 (12) | 0.7405 (3) | 0.55188 (14) | 0.0477 (5) |
| H27 | 0.2049 | 0.8105 | 0.5963 | 0.057* |
| C28 | 0.22735 (11) | 0.7505 (3) | 0.47865 (13) | 0.0461 (5) |
| H28 | 0.2658 | 0.8264 | 0.4741 | 0.055* |
| C29 | 0.20693 (9) | 0.6482 (2) | 0.41146 (11) | 0.0355 (4) |
| N1 | 0.05252 (8) | 0.57835 (19) | 0.14636 (9) | 0.0338 (3) |
| N2 | 0.15442 (8) | 0.44924 (19) | 0.27629 (9) | 0.0348 (3) |
| O1 | −0.07848 (8) | 0.59298 (19) | 0.20016 (11) | 0.0509 (4) |
| H1A | −0.0408 | 0.5489 | 0.1844 | 0.076* |
| O2 | 0.24508 (8) | 0.6613 (2) | 0.34177 (8) | 0.0487 (4) |
| H2A | 0.2264 | 0.6006 | 0.3053 | 0.073* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.0384 (10) | 0.0346 (9) | 0.0407 (9) | −0.0049 (8) | 0.0003 (8) | −0.0001 (8) |
| C2 | 0.0365 (10) | 0.0390 (10) | 0.0591 (12) | −0.0070 (8) | −0.0073 (8) | −0.0052 (9) |
| C3 | 0.0296 (10) | 0.0468 (12) | 0.0742 (14) | −0.0096 (9) | 0.0104 (9) | −0.0005 (11) |
| C4 | 0.0464 (11) | 0.0669 (14) | 0.0487 (11) | −0.0111 (11) | 0.0144 (9) | 0.0084 (11) |
| C5 | 0.0386 (10) | 0.0536 (12) | 0.0374 (9) | −0.0087 (9) | 0.0009 (8) | 0.0026 (9) |
| C6 | 0.0301 (9) | 0.0270 (8) | 0.0383 (9) | −0.0033 (7) | 0.0021 (7) | 0.0017 (7) |
| C7 | 0.0299 (8) | 0.0341 (9) | 0.0280 (8) | −0.0069 (7) | −0.0017 (6) | 0.0013 (6) |
| C8 | 0.0303 (9) | 0.0335 (9) | 0.0311 (8) | −0.0046 (7) | −0.0011 (6) | −0.0007 (7) |
| C9 | 0.0379 (10) | 0.0355 (10) | 0.0462 (10) | −0.0049 (8) | 0.0031 (8) | −0.0008 (8) |
| C10 | 0.0544 (12) | 0.0365 (10) | 0.0526 (12) | 0.0058 (9) | 0.0034 (10) | −0.0034 (9) |
| C11 | 0.0418 (11) | 0.0531 (13) | 0.0513 (12) | 0.0102 (10) | 0.0028 (9) | −0.0072 (10) |
| C12 | 0.0310 (10) | 0.0535 (13) | 0.0494 (11) | −0.0034 (9) | 0.0057 (8) | 0.0002 (9) |
| C13 | 0.0315 (9) | 0.0409 (10) | 0.0389 (9) | −0.0042 (8) | −0.0020 (7) | 0.0016 (8) |
| C14 | 0.0513 (12) | 0.0435 (10) | 0.0391 (9) | −0.0056 (10) | 0.0053 (8) | −0.0027 (9) |
| C15 | 0.0318 (9) | 0.0306 (9) | 0.0372 (9) | −0.0056 (7) | 0.0066 (7) | −0.0007 (7) |
| C16 | 0.0406 (10) | 0.0294 (8) | 0.0391 (9) | −0.0029 (7) | 0.0018 (7) | −0.0018 (7) |
| C17 | 0.0341 (9) | 0.0512 (12) | 0.0492 (11) | −0.0046 (9) | 0.0052 (8) | −0.0058 (9) |
| C18 | 0.0379 (11) | 0.089 (2) | 0.0546 (13) | −0.0233 (12) | 0.0085 (9) | −0.0164 (13) |
| C19 | 0.0761 (18) | 0.0632 (16) | 0.0534 (13) | −0.0401 (15) | 0.0107 (12) | −0.0014 (12) |
| C20 | 0.0856 (19) | 0.0415 (12) | 0.0645 (15) | −0.0188 (13) | 0.0017 (13) | 0.0086 (11) |
| C21 | 0.0495 (12) | 0.0368 (10) | 0.0564 (12) | −0.0059 (9) | −0.0017 (9) | 0.0050 (9) |
| C22 | 0.0328 (9) | 0.0340 (9) | 0.0326 (8) | −0.0063 (7) | 0.0012 (7) | −0.0034 (7) |
| C23 | 0.0263 (8) | 0.0258 (8) | 0.0396 (9) | 0.0011 (6) | −0.0013 (6) | 0.0008 (7) |
| C24 | 0.0260 (8) | 0.0266 (8) | 0.0382 (8) | 0.0013 (6) | −0.0028 (6) | 0.0002 (7) |
| C25 | 0.0309 (9) | 0.0336 (9) | 0.0461 (10) | −0.0024 (8) | 0.0034 (7) | −0.0017 (8) |
| C26 | 0.0419 (10) | 0.0466 (11) | 0.0429 (10) | −0.0020 (9) | 0.0067 (8) | −0.0078 (8) |
| C27 | 0.0472 (11) | 0.0480 (12) | 0.0473 (11) | −0.0063 (10) | −0.0032 (9) | −0.0140 (9) |
| C28 | 0.0404 (10) | 0.0452 (11) | 0.0520 (11) | −0.0149 (9) | −0.0066 (8) | −0.0033 (9) |
| C29 | 0.0307 (9) | 0.0357 (9) | 0.0398 (9) | −0.0026 (8) | −0.0029 (7) | 0.0036 (8) |
| N1 | 0.0307 (7) | 0.0322 (8) | 0.0385 (8) | −0.0061 (6) | 0.0031 (6) | 0.0001 (6) |

| | | | | | | |
|---|---|---|---|---|---|---|
| N2 | 0.0345 (7) | 0.0323 (7) | 0.0376 (7) | −0.0043 (6) | 0.0003 (6) | −0.0011 (6) |
| O1 | 0.0343 (7) | 0.0413 (8) | 0.0778 (11) | −0.0062 (6) | 0.0092 (7) | 0.0116 (8) |
| O2 | 0.0440 (8) | 0.0613 (10) | 0.0410 (7) | −0.0221 (7) | 0.0020 (6) | 0.0007 (7) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| C1—C2 | 1.380 (3) | C15—H15 | 0.98 |
| C1—C6 | 1.385 (3) | C16—N2 | 1.460 (2) |
| C1—H1 | 0.93 | C16—H16A | 0.97 |
| C2—C3 | 1.374 (3) | C16—H16B | 0.97 |
| C2—H2 | 0.93 | C17—C22 | 1.385 (3) |
| C3—C4 | 1.371 (3) | C17—C18 | 1.395 (3) |
| C3—H3 | 0.93 | C17—H17 | 0.93 |
| C4—C5 | 1.391 (3) | C18—C19 | 1.372 (4) |
| C4—H4 | 0.93 | C18—H18 | 0.93 |
| C5—C6 | 1.388 (3) | C19—C20 | 1.369 (4) |
| C5—H5 | 0.93 | C19—H19 | 0.93 |
| C6—C7 | 1.508 (2) | C20—C21 | 1.382 (3) |
| C7—N1 | 1.283 (2) | C20—H20 | 0.93 |
| C7—C8 | 1.469 (3) | C21—C22 | 1.389 (3) |
| C8—C9 | 1.399 (3) | C21—H21 | 0.93 |
| C8—C13 | 1.419 (2) | C22—C23 | 1.500 (2) |
| C9—C10 | 1.378 (3) | C23—N2 | 1.284 (2) |
| C9—H9 | 0.93 | C23—C24 | 1.477 (2) |
| C10—C11 | 1.388 (3) | C24—C25 | 1.399 (2) |
| C10—H10 | 0.93 | C24—C29 | 1.411 (2) |
| C11—C12 | 1.376 (3) | C25—C26 | 1.383 (3) |
| C11—H11 | 0.93 | C25—H25 | 0.93 |
| C12—C13 | 1.389 (3) | C26—C27 | 1.386 (3) |
| C12—H12 | 0.93 | C26—H26 | 0.93 |
| C13—O1 | 1.346 (3) | C27—C28 | 1.376 (3) |
| C14—C15 | 1.525 (3) | C27—H27 | 0.93 |
| C14—H14A | 0.96 | C28—C29 | 1.388 (3) |
| C14—H14B | 0.96 | C28—H28 | 0.93 |
| C14—H14C | 0.96 | C29—O2 | 1.347 (2) |
| C15—N1 | 1.460 (2) | O1—H1A | 0.82 |
| C15—C16 | 1.525 (3) | O2—H2A | 0.82 |
| C2—C1—C6 | 120.49 (18) | C16—C15—H15 | 109.5 |
| C2—C1—H1 | 119.8 | N2—C16—C15 | 109.55 (15) |
| C6—C1—H1 | 119.8 | N2—C16—H16A | 109.8 |
| C3—C2—C1 | 120.01 (18) | C15—C16—H16A | 109.8 |
| C3—C2—H2 | 120 | N2—C16—H16B | 109.8 |
| C1—C2—H2 | 120 | C15—C16—H16B | 109.8 |
| C4—C3—C2 | 120.00 (18) | H16A—C16—H16B | 108.2 |
| C4—C3—H3 | 120 | C22—C17—C18 | 119.5 (2) |
| C2—C3—H3 | 120 | C22—C17—H17 | 120.2 |
| C3—C4—C5 | 120.72 (19) | C18—C17—H17 | 120.2 |
| C3—C4—H4 | 119.6 | C19—C18—C17 | 120.0 (2) |
| C5—C4—H4 | 119.6 | C19—C18—H18 | 120 |

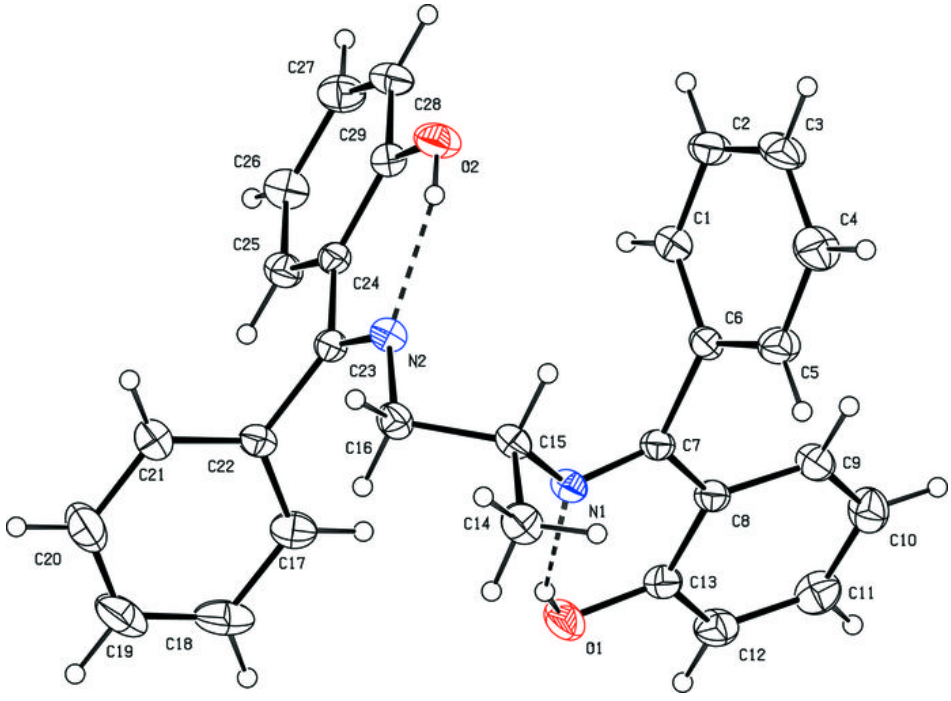
| | | | |
|---|---|---|---|
| C6—C5—C4 | 119.26 (18) | C17—C18—H18 | 120 |
| C6—C5—H5 | 120.4 | C20—C19—C18 | 120.5 (2) |
| C4—C5—H5 | 120.4 | C20—C19—H19 | 119.7 |
| C1—C6—C5 | 119.48 (17) | C18—C19—H19 | 119.7 |
| C1—C6—C7 | 118.56 (16) | C19—C20—C21 | 120.3 (2) |
| C5—C6—C7 | 121.90 (16) | C19—C20—H20 | 119.9 |
| N1—C7—C8 | 119.60 (16) | C21—C20—H20 | 119.9 |
| N1—C7—C6 | 122.34 (17) | C20—C21—C22 | 119.8 (2) |
| C8—C7—C6 | 118.02 (15) | C20—C21—H21 | 120.1 |
| C9—C8—C13 | 117.66 (17) | C22—C21—H21 | 120.1 |
| C9—C8—C7 | 121.20 (17) | C17—C22—C21 | 119.81 (18) |
| C13—C8—C7 | 121.13 (15) | C17—C22—C23 | 121.07 (18) |
| C10—C9—C8 | 122.01 (19) | C21—C22—C23 | 119.12 (16) |
| C10—C9—H9 | 119 | N2—C23—C24 | 118.18 (15) |
| C8—C9—H9 | 119 | N2—C23—C22 | 123.25 (16) |
| C9—C10—C11 | 119.3 (2) | C24—C23—C22 | 118.55 (15) |
| C9—C10—H10 | 120.4 | C25—C24—C29 | 117.87 (16) |
| C11—C10—H10 | 120.4 | C25—C24—C23 | 121.07 (15) |
| C12—C11—C10 | 120.5 (2) | C29—C24—C23 | 121.06 (15) |
| C12—C11—H11 | 119.8 | C26—C25—C24 | 121.64 (18) |
| C10—C11—H11 | 119.8 | C26—C25—H25 | 119.2 |
| C11—C12—C13 | 120.7 (2) | C24—C25—H25 | 119.2 |
| C11—C12—H12 | 119.6 | C25—C26—C27 | 119.29 (19) |
| C13—C12—H12 | 119.6 | C25—C26—H26 | 120.4 |
| O1—C13—C12 | 118.80 (18) | C27—C26—H26 | 120.4 |
| O1—C13—C8 | 121.39 (17) | C28—C27—C26 | 120.58 (19) |
| C12—C13—C8 | 119.81 (18) | C28—C27—H27 | 119.7 |
| C15—C14—H14A | 109.5 | C26—C27—H27 | 119.7 |
| C15—C14—H14B | 109.5 | C27—C28—C29 | 120.45 (19) |
| H14A—C14—H14B | 109.5 | C27—C28—H28 | 119.8 |
| C15—C14—H14C | 109.5 | C29—C28—H28 | 119.8 |
| H14A—C14—H14C | 109.5 | O2—C29—C28 | 117.95 (17) |
| H14B—C14—H14C | 109.5 | O2—C29—C24 | 121.87 (16) |
| N1—C15—C14 | 108.39 (15) | C28—C29—C24 | 120.17 (17) |
| N1—C15—C16 | 109.14 (14) | C7—N1—C15 | 122.13 (16) |
| C14—C15—C16 | 110.66 (15) | C23—N2—C16 | 121.53 (16) |
| N1—C15—H15 | 109.5 | C13—O1—H1A | 109.5 |
| C14—C15—H15 | 109.5 | C29—O2—H2A | 109.5 |
| C6—C1—C2—C3 | 2.0 (3) | C19—C20—C21—C22 | −0.1 (4) |
| C1—C2—C3—C4 | −0.7 (3) | C18—C17—C22—C21 | 0.4 (3) |
| C2—C3—C4—C5 | −0.5 (4) | C18—C17—C22—C23 | 179.17 (18) |
| C3—C4—C5—C6 | 0.5 (4) | C20—C21—C22—C17 | −0.2 (3) |
| C2—C1—C6—C5 | −1.9 (3) | C20—C21—C22—C23 | −179.00 (19) |
| C2—C1—C6—C7 | 175.34 (18) | C17—C22—C23—N2 | −93.9 (2) |
| C4—C5—C6—C1 | 0.7 (3) | C21—C22—C23—N2 | 84.9 (2) |
| C4—C5—C6—C7 | −176.5 (2) | C17—C22—C23—C24 | 87.8 (2) |
| C1—C6—C7—N1 | −87.8 (2) | C21—C22—C23—C24 | −93.4 (2) |
| C5—C6—C7—N1 | 89.5 (2) | N2—C23—C24—C25 | 172.54 (17) |
| C1—C6—C7—C8 | 89.8 (2) | C22—C23—C24—C25 | −9.1 (2) |

| | | | |
|---|---|---|---|
| C5—C6—C7—C8 | −92.9 (2) | N2—C23—C24—C29 | −7.8 (2) |
| N1—C7—C8—C9 | −171.73 (18) | C22—C23—C24—C29 | 170.61 (16) |
| C6—C7—C8—C9 | 10.6 (2) | C29—C24—C25—C26 | 0.5 (3) |
| N1—C7—C8—C13 | 7.3 (3) | C23—C24—C25—C26 | −179.84 (18) |
| C6—C7—C8—C13 | −170.35 (16) | C24—C25—C26—C27 | 0.3 (3) |
| C13—C8—C9—C10 | 0.1 (3) | C25—C26—C27—C28 | −0.9 (3) |
| C7—C8—C9—C10 | 179.19 (17) | C26—C27—C28—C29 | 0.7 (3) |
| C8—C9—C10—C11 | 1.1 (3) | C27—C28—C29—O2 | −178.9 (2) |
| C9—C10—C11—C12 | −0.7 (3) | C27—C28—C29—C24 | 0.2 (3) |
| C10—C11—C12—C13 | −0.8 (3) | C25—C24—C29—O2 | 178.35 (17) |
| C11—C12—C13—O1 | −178.8 (2) | C23—C24—C29—O2 | −1.4 (3) |
| C11—C12—C13—C8 | 2.0 (3) | C25—C24—C29—C28 | −0.7 (3) |
| C9—C8—C13—O1 | 179.18 (19) | C23—C24—C29—C28 | 179.59 (17) |
| C7—C8—C13—O1 | 0.1 (3) | C8—C7—N1—C15 | 177.40 (14) |
| C9—C8—C13—C12 | −1.7 (3) | C6—C7—N1—C15 | −5.0 (3) |
| C7—C8—C13—C12 | 179.27 (17) | C14—C15—N1—C7 | −111.3 (2) |
| N1—C15—C16—N2 | −66.08 (18) | C16—C15—N1—C7 | 128.14 (18) |
| C14—C15—C16—N2 | 174.74 (15) | C24—C23—N2—C16 | −175.93 (15) |
| C22—C17—C18—C19 | −0.2 (3) | C22—C23—N2—C16 | 5.8 (3) |
| C17—C18—C19—C20 | −0.1 (4) | C15—C16—N2—C23 | 131.47 (17) |
| C18—C19—C20—C21 | 0.3 (4) | | |

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1—H1A···N1 | 0.82 | 1.84 | 2.573 (2) | 147 |
| O2—H2A···N2 | 0.82 | 1.83 | 2.553 (2) | 147 |

**Fig. 1**


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