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2,2′-[(2,2′-Bipyridine-3,3′-diyl)bis(nitrilomethylidyne)]diphenol

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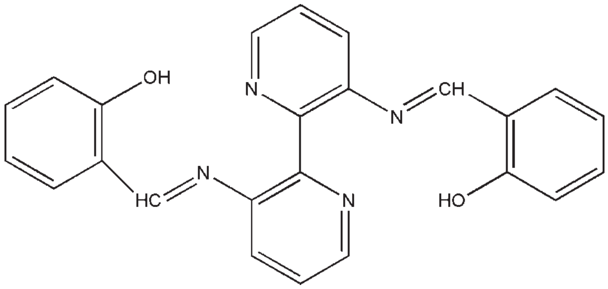
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.004 Å; R factor = 0.055; wR factor = 0.143; data-to-parameter ratio = 14.0.

The title molecule, $C_{24}H_{18}N_4O_2$, lies on a twofold rotation axis with a dihedral angle of 73.7 (1)° between the mean planes of the symmetry-related pyridine rings. The dihedral angle between unique benzene and pyridine rings is 8.0 (1)°. An intramolecular O—H···N hydrogen bond may influence the molecular conformation. In the crystal structure, there are weak π–π stacking interactions with a centroid–centroid distance of 3.7838 (15) Å.

Related literature

For background to the use of 2,2-bipyridine derivatives in coordination chemistry, see: Stephenson & Hardie (2007); Hou *et al.* (2008*a*,*b*). For a related structure, see: Rice *et al.* (2002).



Experimental

Crystal data

$C_{24}H_{18}N_4O_2$
M_r = 394.42
Monoclinic, $C2/c$
a = 21.017 (3) Å
b = 8.4485 (14) Å
c = 13.012 (2) Å
β = 121.980 (3)°
V = 1959.8 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 298 K
0.38 × 0.20 × 0.16 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.967, T_{max} = 0.986
5242 measured reflections
1913 independent reflections
1334 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.143
S = 1.02
1913 reflections
137 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.13 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1	0.82	1.89	2.619 (2)	147

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2878).

References

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supplementary materials

Acta Cryst. (2009). E**65**, o2290   [**doi:10.1107/S1600536809032346**]

2,2'-[(2,2'-Bipyridine-3,3'-diyl)bis(nitrilomethylidyne)]diphenol

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Comment

Derivatives of 2,2-bipyridine are useful ligands and play an important role in modern coordination chemistry (Stephenson & Hardie, 2007; Hou *et al.*, 2008*a*,*b*). The title compound (I) was synthesized as a potential ligand and its crystal structure is reported herein. The molecular structure of (I) is shown in Fig. 1. The molecule lies on a twofold rotation axis with dihedral angle of 73.7 (1)° between the mean planes of the symmetry related pyridine rings. In the related crystal structure of 3,3'-diamino-2,2'-dipyridine which has already been reported (Rice *et al.* 2002) the molecule lies on an inversion center and the mean planes of the two pyridine are essentially co-planar. The large deviation from planarity in (I) can be expected in terms of steric relief with respect to the bulky 2-(methylimino)phenol substituents. An intramolecular O—H···N hydrogen bond may influence the molecular conformation. In the crystal structure, there is a weak π–π stacking interactions involving pyridine rings and symmetry-related benzene rings with the relevant geometry being $Cg1\cdots Cg2^{i}$ = 3.7838 (15) Å, $Cg1\cdots Cg2^{i}_{perp}$ = 3.353 Å and α = 7.97° [symmetry code: (i) -*x*, 1-*y*, -*z*; *Cg*1 and *Cg*2 are the centroids of the C8—C12/N2 ring and C1—C6 ring, respectively; $Cg1\cdots Cg2^{1}_{perp}$ is the perpendicular distance from ring *Cg*1 to ring $Cg2^{i}$; α is the dihedral between ring plane *Cg*1 and ring plane $Cg2^{i}$].

Experimental

A 35 ml methanol solution of 3,3'-diamino-2,2'-dipyridine (1.03 g, 5.53 mmol) was added to salicylaldehyde (1.40 g, 11.46 mmol) and the mixture was stirred and refluxed for 5 h. Yellow single crystals were obtained after the filtrate had been allowed to stand at room temperature for three weeks.

Refinement

All H atoms were placed in in calculated positions and refined as riding with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C), O—H = 0.82 Å and U_{iso}(H) = 1.5U_{eq}(O).

Figures

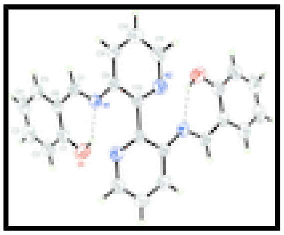

Fig. 1. The molecular structure of the title compound with displacement ellipsoids drawn at the 30% probability level. The dashed lines indicate hydrogen bonds and the unlabeled atoms are related by the symmetry code (-x, y, -z+1/2).

2,2'-[(2,2'-Bipyridine-3,3'-diyl)bis(nitrilomethylidyne)]diphenol

Crystal data

$C_{24}H_{18}N_4O_2$

$M_r = 394.42$

Monoclinic, $C2/c$

Hall symbol: -C 2yc

$a = 21.017$ (3) Å

$b = 8.4485$ (14) Å

$c = 13.012$ (2) Å

$\beta = 121.980$ (3)°

$V = 1959.8$ (5) Å^3

$Z = 4$

$F_{000} = 824$

$D_x = 1.337$ Mg m^{-3}

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 1047 reflections

$\theta = 2.7$–22.4°

$\mu = 0.09$ mm^{-1}

$T = 298$ K

Block, yellow

0.38 × 0.20 × 0.16 mm

Data collection

Bruker SMART CCD diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 298$ K

φ and ω scans

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)

$T_{min} = 0.967$, $T_{max} = 0.986$

5242 measured reflections

1913 independent reflections

1334 reflections with $I > 2\sigma(I)$

$R_{int} = 0.025$

$\theta_{max} = 26.0$°

$\theta_{min} = 2.3$°

$h = -21 \rightarrow 25$

$k = -9 \rightarrow 10$

$l = -15 \rightarrow 16$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.055$

$wR(F^2) = 0.143$

$S = 1.02$

1913 reflections

137 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.063P)^2 + 0.6383P]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.17$ e Å^{-3}

$\Delta\rho_{min} = -0.13$ e Å^{-3}

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	$U_{\rm iso}$*/$U_{\rm eq}$
C1	0.12783 (13)	0.8486 (3)	0.1341 (2)	0.0702 (6)
C2	0.18125 (15)	0.9514 (3)	0.1412 (3)	0.0917 (8)
H2	0.2263	0.9648	0.2147	0.110*
C3	0.16874 (18)	1.0339 (3)	0.0413 (3)	0.0928 (9)
H3	0.2052	1.1029	0.0480	0.111*
C4	0.10274 (19)	1.0156 (3)	−0.0687 (3)	0.0867 (8)
H4	0.0946	1.0706	−0.1366	0.104*
C5	0.04893 (14)	0.9146 (3)	−0.0766 (2)	0.0709 (6)
H5	0.0042	0.9023	−0.1507	0.085*
C6	0.05958 (12)	0.8302 (2)	0.02338 (19)	0.0567 (5)
C7	0.00038 (11)	0.7307 (2)	0.01146 (18)	0.0553 (5)
H7	−0.0435	0.7208	−0.0642	0.066*
C8	−0.05332 (10)	0.5646 (2)	0.09104 (17)	0.0513 (5)
C9	−0.12535 (12)	0.5543 (3)	−0.01036 (19)	0.0666 (6)
H9	−0.1379	0.6077	−0.0812	0.080*
C10	−0.17782 (13)	0.4647 (3)	−0.0050 (2)	0.0723 (6)
H10	−0.2263	0.4563	−0.0722	0.087*
C11	−0.15804 (12)	0.3878 (3)	0.1000 (2)	0.0681 (6)
H11	−0.1942	0.3269	0.1019	0.082*
C12	−0.03848 (11)	0.4816 (2)	0.19397 (17)	0.0516 (5)
N1	0.00610 (9)	0.65566 (19)	0.10122 (14)	0.0549 (4)
N2	−0.08982 (9)	0.3951 (2)	0.20004 (15)	0.0621 (5)
O1	0.14272 (9)	0.7671 (3)	0.23344 (14)	0.0978 (6)
H1	0.1053	0.7176	0.2190	0.147*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0733 (15)	0.0801 (15)	0.0708 (16)	−0.0074 (12)	0.0475 (13)	−0.0130 (12)
C2	0.0844 (19)	0.105 (2)	0.102 (2)	−0.0209 (15)	0.0600 (17)	−0.0259 (17)
C3	0.107 (2)	0.0738 (17)	0.142 (3)	−0.0137 (15)	0.097 (2)	−0.0202 (18)
C4	0.121 (2)	0.0668 (16)	0.119 (2)	0.0108 (15)	0.096 (2)	0.0133 (15)
C5	0.0889 (16)	0.0662 (14)	0.0815 (16)	0.0107 (12)	0.0614 (14)	0.0075 (12)
C6	0.0717 (14)	0.0539 (12)	0.0624 (13)	0.0046 (9)	0.0477 (12)	−0.0032 (10)
C7	0.0638 (12)	0.0581 (12)	0.0522 (12)	0.0057 (9)	0.0363 (10)	−0.0029 (9)
C8	0.0561 (12)	0.0530 (11)	0.0510 (12)	0.0017 (9)	0.0327 (10)	−0.0056 (9)
C9	0.0669 (14)	0.0753 (15)	0.0553 (13)	0.0011 (11)	0.0308 (11)	0.0047 (11)

C10	0.0587 (13)	0.0854 (16)	0.0628 (14)	−0.0059 (11)	0.0255 (11)	−0.0063 (12)
C11	0.0602 (13)	0.0752 (15)	0.0751 (15)	−0.0104 (11)	0.0401 (12)	−0.0098 (12)
C12	0.0569 (12)	0.0538 (11)	0.0544 (12)	0.0000 (9)	0.0364 (9)	−0.0069 (9)
N1	0.0613 (10)	0.0588 (10)	0.0524 (10)	0.0019 (8)	0.0353 (8)	0.0009 (8)
N2	0.0619 (11)	0.0686 (11)	0.0634 (11)	−0.0071 (9)	0.0385 (9)	−0.0041 (9)
O1	0.0857 (13)	0.1405 (17)	0.0616 (11)	−0.0203 (11)	0.0352 (9)	0.0015 (10)

Geometric parameters (Å, °)

C1—O1	1.347 (3)	C7—H7	0.9300
C1—C2	1.383 (3)	C8—C9	1.387 (3)
C1—C6	1.403 (3)	C8—C12	1.393 (3)
C2—C3	1.372 (4)	C8—N1	1.412 (2)
C2—H2	0.9300	C9—C10	1.369 (3)
C3—C4	1.376 (4)	C9—H9	0.9300
C3—H3	0.9300	C10—C11	1.364 (3)
C4—C5	1.377 (3)	C10—H10	0.9300
C4—H4	0.9300	C11—N2	1.333 (3)
C5—C6	1.393 (3)	C11—H11	0.9300
C5—H5	0.9300	C12—N2	1.340 (2)
C6—C7	1.440 (3)	C12—C12$^{\text{i}}$	1.498 (4)
C7—N1	1.278 (2)	O1—H1	0.8200
O1—C1—C2	119.3 (2)	C6—C7—H7	118.9
O1—C1—C6	121.3 (2)	C9—C8—C12	117.31 (18)
C2—C1—C6	119.4 (2)	C9—C8—N1	126.07 (18)
C3—C2—C1	120.9 (3)	C12—C8—N1	116.59 (17)
C3—C2—H2	119.5	C10—C9—C8	119.3 (2)
C1—C2—H2	119.5	C10—C9—H9	120.4
C2—C3—C4	120.7 (3)	C8—C9—H9	120.4
C2—C3—H3	119.7	C11—C10—C9	119.2 (2)
C4—C3—H3	119.7	C11—C10—H10	120.4
C3—C4—C5	118.9 (3)	C9—C10—H10	120.4
C3—C4—H4	120.6	N2—C11—C10	123.8 (2)
C5—C4—H4	120.6	N2—C11—H11	118.1
C4—C5—C6	121.9 (2)	C10—C11—H11	118.1
C4—C5—H5	119.1	N2—C12—C8	123.65 (18)
C6—C5—H5	119.1	N2—C12—C12$^{\text{i}}$	115.52 (18)
C5—C6—C1	118.2 (2)	C8—C12—C12$^{\text{i}}$	120.82 (18)
C5—C6—C7	119.7 (2)	C7—N1—C8	122.31 (17)
C1—C6—C7	122.05 (19)	C11—N2—C12	116.79 (18)
N1—C7—C6	122.25 (19)	C1—O1—H1	109.5
N1—C7—H7	118.9		
O1—C1—C2—C3	178.6 (2)	N1—C8—C9—C10	−177.84 (18)
C6—C1—C2—C3	−0.8 (4)	C8—C9—C10—C11	0.1 (3)
C1—C2—C3—C4	−0.3 (4)	C9—C10—C11—N2	0.5 (3)
C2—C3—C4—C5	0.8 (4)	C9—C8—C12—N2	−0.7 (3)
C3—C4—C5—C6	−0.2 (3)	N1—C8—C12—N2	177.33 (16)
C4—C5—C6—C1	−0.9 (3)	C9—C8—C12—C12$^{\text{i}}$	177.85 (16)

C4—C5—C6—C7	177.60 (19)	N1—C8—C12—C12^{i}	−4.1 (2)
O1—C1—C6—C5	−178.0 (2)	C6—C7—N1—C8	176.66 (16)
C2—C1—C6—C5	1.4 (3)	C9—C8—N1—C7	−5.5 (3)
O1—C1—C6—C7	3.5 (3)	C12—C8—N1—C7	176.58 (17)
C2—C1—C6—C7	−177.06 (19)	C10—C11—N2—C12	−1.1 (3)
C5—C6—C7—N1	−177.25 (18)	C8—C12—N2—C11	1.3 (3)
C1—C6—C7—N1	1.2 (3)	C12^{i}—C12—N2—C11	−177.40 (16)
C12—C8—C9—C10	0.0 (3)		

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1	0.82	1.89	2.619 (2)	147

Fig. 1