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N,*N*′-Bis[(2-phenyl-2*H*-1,2,3-triazol-4-yl)methylidene]benzene-1,4-diamine

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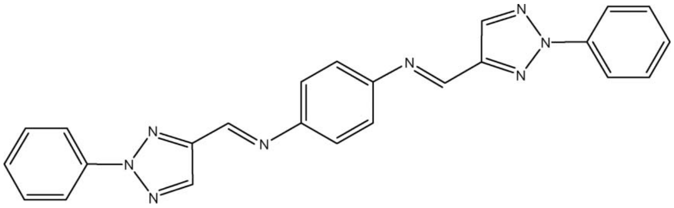
Key indicators: single-crystal X-ray study; T = 153 K; mean σ(C–C) = 0.002 Å; R factor = 0.041; wR factor = 0.120; data-to-parameter ratio = 15.6.

The centrosymmetric title compound, $C_{24}H_{18}N_8$, was prepared by reaction of 2-phenyl-1,2,3-triazole-4-carbaldehyde with 1,4-phenylenediamine. The dihedral angle between the outer phenyl ring and the triazole ring is 6.9 (3)°. The crystal structure is stabilized by intermolecular aromatic π–π interactions between the parallel triazole and benzene rings [the centroid–centroid separation is 3.485 (2) Å].

Related literature

For related literature, see: Li *et al.* (2006); Yan *et al.* (2005); Klingele & Brooker (2004).



Experimental

Crystal data

$C_{24}H_{18}N_8$
M_r = 418.46
Monoclinic, $P2_1/c$
a = 17.670 (4) Å
b = 4.800 (1) Å
c = 11.751 (2) Å
β = 94.42 (3)°
V = 993.7 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 153 (2) K
0.45 × 0.40 × 0.35 mm

Data collection

Rigaku R-AXIS SPIDER diffractometer
Absorption correction: none
8889 measured reflections
2273 independent reflections
1743 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.032

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.120
S = 1.02
2273 reflections
146 parameters
H-atom parameters constrained
$\Delta\rho_{\rm max}$ = 0.23 e Å^{-3}
$\Delta\rho_{\rm min}$ = −0.24 e Å^{-3}

Data collection: *RAPID-AUTO* (Rigaku, 2004); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *DIAMOND* (Brandenburg, 1998); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LX2008).

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supplementary materials

Acta Cryst. (2007). E**63**, o2934 [**doi:10.1107/S1600536807022830**]

N,*N*'-Bis[(2-phenyl-2*H*-1,2,3-triazol-4-yl)methylidene]benzene-1,4-diamine

J. Hu, **Z.-F. Xie** and **F.-M. Liu**

Comment

Aromatic nitrogen heterocycles are arguably the most facile and ligands used widely in coordination chemistry. Ligands based on heterocycles containing more than one nitrogen atom within the aromatic ring are capable of forming oligo- and polynuclear coordination compounds by bridging metal centres (Klingele et al., 2004). Schiff bases are condensation products of arylamines and carbonyl compounds. Unlike the aliphatic imines, these compounds are quite stable and represent versatile intermediates for preparation of a number of industrial and biological compounds, for example, arendiazonium nitrates, N-arylarencarboxamides, corresponding amines and cyanoamines, beta-lactams (Yan et al.,2005). 1,2,3-triazole and its derivatives are important in the synthesis of heteroarmatic compounds.

We report here the crystal structure of (I) (Fig. 1), synthesized by the reaction of 1,4-phenylene diamine with 2-phenyl-1,2,3-triazol-4-carbaldehyde. The bond lengths and angles in the (I), show normal values. In the crystal structure, π—π stacking interactions are observed between adjacent molecules, which is parallel (Fig. 2). The $Cg1\cdots Cg2^{iv}$ distance is 3.485 (2) Å (Cg1 and Cg2 are the centroids of the N1,N2/C7,C8/N3 and C1—C6 rings; symmetry code as in Fig. 2).

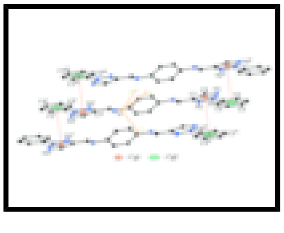
Experimental

Two drops of glacial acetic acid were added to a solution of 2-phenyl-1,2,3-triazole-4-carbaldehyde (0.346 g, 2 mmol) (Li *et al.*, 2006) in absolute ethanol (20 ml), then dropwised 1,4-phenylene diamine (0.108 g, 1 mmol) in absolute ethanol (10 ml). The reaction mixture was refluxed for 0.5 hr., after cooling to room temperature,the precipitates were filtered and recrystallized: yield 91%, m.p. 475 K. Single-crystals were grown from a mixture solution of ethyl acetate and petroleum ether by slow evaporation.

Refinement

All H atoms were positioned geometrically and refined using a riding model, with C—H = 0.95 Å and $U_{iso}(H) = 1.2U_{eq}(C)$.

Figures



N,*N*'-Bis[(2-phenyl-2*H*-1,2,3-triazol-4-yl)methylidene]benzene-1,4-diamine

Crystal data

$C_{24}H_{18}N_8$

$M_r = 418.46$

Monoclinic, $P2_1/c$

Hall symbol: -p 2ybc

$a = 17.670$ (4) Å

$b = 4.800$ (1) Å

$c = 11.751$ (2) Å

$\beta = 94.42$ (3)°

$V = 993.7$ (4) Å^3

$Z = 2$

$F_{000} = 436$

$D_x = 1.399$ Mg m^{-3}

Melting point: 475 K

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

Cell parameters from 6687 reflections

$\theta = 3.5$–27.5°

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

$T = 153$ (2) K

Sheet, light yellow

0.45 × 0.40 × 0.35 mm

Data collection

Rigaku R-AXIS SPIDER diffractometer

Radiation source: Rotating Anode

Monochromator: graphite

$T = 153(2)$ K

ω scans

Absorption correction: none

8889 measured reflections

2273 independent reflections

1743 reflections with $I > 2\sigma(I)$

$R_{\rm int} = 0.032$

$\theta_{\rm max} = 27.5°$

$\theta_{\rm min} = 3.5°$

$h = -22 \rightarrow 22$

$k = -6 \rightarrow 6$

$l = -12 \rightarrow 15$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.041$

$wR(F^2) = 0.120$

$S = 1.02$

2273 reflections

146 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

$w = 1/[\sigma^2(F_o^2) + (0.0729P)^2 + 0.1883P]$
where $P = (F_o^2 + 2F_c^2)/3$

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

$\Delta\rho_{\rm max} = 0.23$ e Å^{-3}

$\Delta\rho_{\rm min} = -0.24$ e Å^{-3}

Extinction correction: SHELXL97,
$Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.026 (5)

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 $F^2 > 2\mathrm{sigma}(F^2)$ 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*	$U_{\rm iso}$*/$U_{\rm eq}$
N1	0.26955 (6)	0.5600 (2)	0.66669 (10)	0.0280 (3)
N2	0.22887 (6)	0.4250 (3)	0.58394 (10)	0.0306 (3)
N3	0.25656 (7)	0.4830 (3)	0.77298 (10)	0.0370 (3)
N4	0.09621 (6)	−0.1206 (3)	0.62525 (10)	0.0310 (3)
C1	0.37153 (7)	0.8752 (3)	0.73231 (13)	0.0347 (3)
H1A	0.3673	0.8152	0.8086	0.042*
C2	0.42482 (7)	1.0749 (3)	0.70784 (14)	0.0370 (4)
H2B	0.4571	1.1525	0.7680	0.044*
C3	0.43132 (8)	1.1617 (3)	0.59726 (14)	0.0381 (4)
H3B	0.4684	1.2965	0.5811	0.046*
C4	0.38356 (8)	1.0513 (4)	0.51003 (14)	0.0405 (4)
H4B	0.3874	1.1135	0.4339	0.049*
C5	0.33006 (7)	0.8506 (3)	0.53232 (13)	0.0357 (4)
H5A	0.2977	0.7737	0.4720	0.043*
C6	0.32462 (6)	0.7647 (3)	0.64333 (12)	0.0280 (3)
C7	0.18671 (7)	0.2479 (3)	0.63998 (11)	0.0288 (3)
C8	0.20430 (7)	0.2846 (3)	0.75709 (12)	0.0357 (3)
H8A	0.1824	0.1840	0.8159	0.043*
C9	0.13538 (7)	0.0576 (3)	0.57624 (12)	0.0313 (3)
H9A	0.1311	0.0673	0.4952	0.038*
C10	0.04894 (7)	−0.3064 (3)	0.55821 (12)	0.0277 (3)
C11	0.05561 (7)	−0.3664 (3)	0.44302 (12)	0.0309 (3)
H11A	0.0938	−0.2770	0.4036	0.037*
C12	−0.00713 (7)	−0.4452 (3)	0.61426 (12)	0.0291 (3)
H12A	−0.0120	−0.4095	0.6929	0.035*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0292 (5)	0.0276 (7)	0.0271 (6)	0.0006 (4)	0.0011 (4)	−0.0024 (5)
N2	0.0324 (5)	0.0279 (7)	0.0312 (7)	−0.0011 (4)	0.0000 (4)	−0.0033 (5)
N3	0.0419 (6)	0.0401 (8)	0.0293 (7)	−0.0083 (5)	0.0041 (5)	−0.0032 (5)

N4	0.0298 (5)	0.0277 (7)	0.0358 (7)	−0.0014 (4)	0.0038 (4)	−0.0062 (5)
C1	0.0352 (7)	0.0353 (8)	0.0334 (8)	−0.0030 (6)	0.0005 (5)	−0.0005 (6)
C2	0.0334 (7)	0.0337 (9)	0.0433 (9)	−0.0031 (5)	−0.0010 (5)	−0.0044 (6)
C3	0.0348 (7)	0.0319 (8)	0.0482 (9)	−0.0032 (6)	0.0078 (6)	−0.0022 (7)
C4	0.0453 (8)	0.0402 (10)	0.0369 (8)	−0.0043 (6)	0.0084 (6)	0.0037 (7)
C5	0.0367 (7)	0.0369 (9)	0.0333 (8)	−0.0024 (6)	0.0019 (5)	−0.0023 (6)
C6	0.0258 (6)	0.0231 (7)	0.0353 (8)	0.0028 (5)	0.0032 (5)	−0.0020 (5)
C7	0.0271 (6)	0.0249 (7)	0.0345 (8)	0.0017 (5)	0.0032 (5)	−0.0013 (5)
C8	0.0378 (7)	0.0368 (9)	0.0331 (8)	−0.0063 (6)	0.0069 (5)	−0.0026 (6)
C9	0.0341 (7)	0.0269 (8)	0.0325 (8)	−0.0005 (5)	0.0004 (5)	−0.0027 (6)
C10	0.0279 (6)	0.0229 (7)	0.0324 (7)	0.0020 (5)	0.0022 (5)	−0.0017 (5)
C11	0.0313 (6)	0.0281 (8)	0.0339 (8)	−0.0017 (5)	0.0076 (5)	−0.0013 (6)
C12	0.0341 (6)	0.0259 (7)	0.0278 (7)	0.0016 (5)	0.0055 (5)	−0.0022 (5)

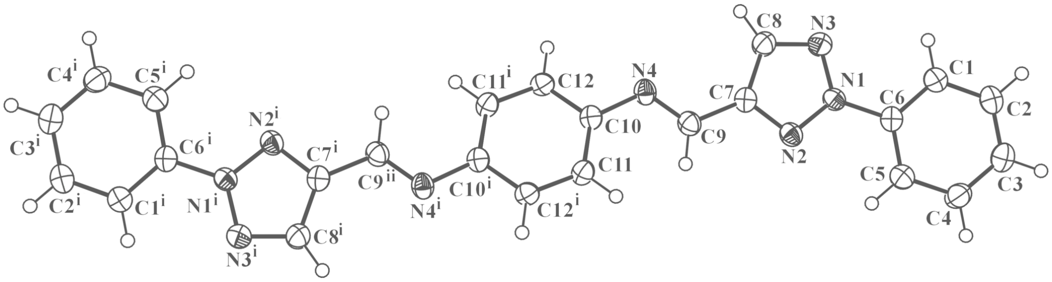
Geometric parameters (Å, °)

N1—N2	1.332 (2)	C4—C5	1.389 (2)
N1—N3	1.339 (2)	C4—H4B	0.9500
N1—C6	1.424 (2)	C5—C6	1.379 (2)
N2—C7	1.337 (2)	C5—H5A	0.9500
N3—C8	1.329 (2)	C7—C8	1.398 (2)
N4—C9	1.267 (2)	C7—C9	1.4534 (19)
N4—C10	1.419 (2)	C8—H8A	0.9500
C1—C6	1.389 (2)	C9—H9A	0.9500
C1—C2	1.389 (2)	C10—C11	1.398 (2)
C1—H1A	0.9500	C10—C12	1.400 (2)
C2—C3	1.378 (2)	C11—C12^{i}	1.384 (2)
C2—H2B	0.9500	C11—H11A	0.9500
C3—C4	1.382 (2)	C12—C11^{i}	1.384 (2)
C3—H3B	0.9500	C12—H12A	0.9500
N2—N1—N3	115.1 (1)	C5—C6—C1	121.1 (1)
N2—N1—C6	122.2 (1)	C5—C6—N1	119.2 (1)
N3—N1—C6	122.6 (1)	C1—C6—N1	119.7 (1)
N1—N2—C7	103.9 (1)	N2—C7—C8	108.3 (1)
C8—N3—N1	103.5 (1)	N2—C7—C9	119.7 (1)
C9—N4—C10	119.4 (1)	C8—C7—C9	132.0 (1)
C6—C1—C2	118.9 (1)	N3—C8—C7	109.1 (1)
C6—C1—H1A	120.6	N3—C8—H8A	125.4
C2—C1—H1A	120.6	C7—C8—H8A	125.4
C3—C2—C1	120.7 (1)	N4—C9—C7	122.1 (1)
C3—C2—H2B	119.6	N4—C9—H9A	119.0
C1—C2—H2B	119.6	C7—C9—H9A	119.0
C2—C3—C4	119.5 (1)	C11—C10—C12	118.3 (1)
C2—C3—H3B	120.2	C11—C10—N4	125.3 (1)
C4—C3—H3B	120.2	C12—C10—N4	116.5 (1)
C3—C4—C5	120.8 (2)	C12^{i}—C11—C10	120.7 (1)
C3—C4—H4B	119.6	C12^{i}—C11—H11A	119.7
C5—C4—H4B	119.6	C10—C11—H11A	119.7

C6—C5—C4	119.0 (1)	$C11^{i}$—C12—C10	121.1 (1)
C6—C5—H5A	120.5	$C11^{i}$—C12—H12A	119.5
C4—C5—H5A	120.5	C10—C12—H12A	119.5
N3—N1—N2—C7	−0.15 (14)	N3—N1—C6—C1	5.34 (19)
C6—N1—N2—C7	177.84 (11)	N1—N2—C7—C8	−0.03 (14)
N2—N1—N3—C8	0.26 (16)	N1—N2—C7—C9	−178.61 (11)
C6—N1—N3—C8	−177.72 (12)	N1—N3—C8—C7	−0.26 (16)
C6—C1—C2—C3	−0.2 (2)	N2—C7—C8—N3	0.19 (16)
C1—C2—C3—C4	0.9 (2)	C9—C7—C8—N3	178.54 (14)
C2—C3—C4—C5	−1.1 (2)	C10—N4—C9—C7	−178.01 (12)
C3—C4—C5—C6	0.7 (2)	N2—C7—C9—N4	177.51 (12)
C4—C5—C6—C1	0.0 (2)	C8—C7—C9—N4	−0.7 (2)
C4—C5—C6—N1	179.65 (12)	C9—N4—C10—C11	18.5 (2)
C2—C1—C6—C5	−0.2 (2)	C9—N4—C10—C12	−163.55 (12)
C2—C1—C6—N1	−179.90 (12)	C12—C10—C11—$C12^{i}$	1.0 (2)
N2—N1—C6—C5	7.83 (18)	N4—C10—C11—$C12^{i}$	179.00 (12)
N3—N1—C6—C5	−174.33 (12)	C11—C10—C12—$C11^{i}$	−1.0 (2)
N2—N1—C6—C1	−172.50 (12)	N4—C10—C12—$C11^{i}$	−179.18 (12)

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

Fig. 1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C12
C12i
C11
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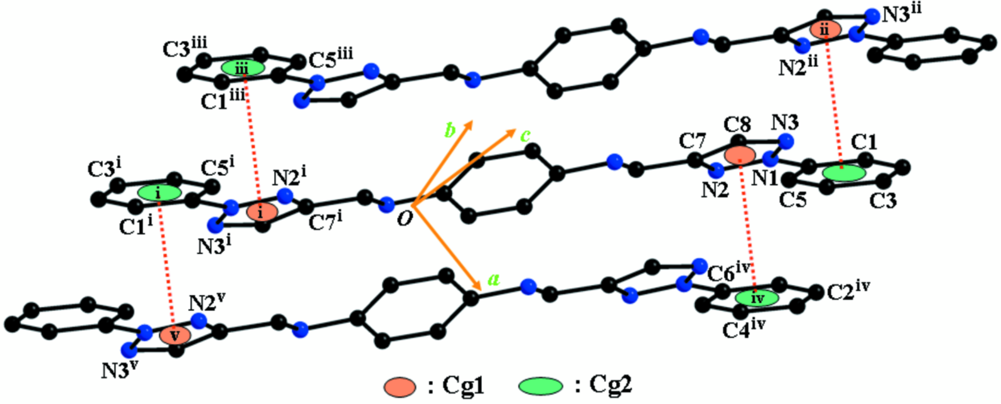
Fig. 2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c
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C8
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C1
N1
N2
C5
C3
C3^{i}
C5^{i}
N2^{i}
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N3^{i}
C7^{i}
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C6^{iv}
iv
C2^{iv}
C4^{iv}
N2^{v}
v
N3^{v}
: Cg1
: Cg2