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4,4′-Bis(1,2,4-triazol-1-ylmethyl)biphenyl

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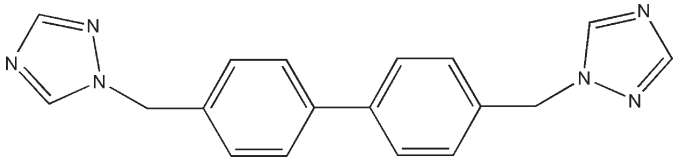
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.003 Å; R factor = 0.042; wR factor = 0.107; data-to-parameter ratio = 12.9.

In the title compound, $C_{18}H_{16}N_6$, the complete molecule is generated by crystallographic inversion symmetry. The dihedral angle between the benzene and triazole rings is 84.1 (3)°. The crystal structure is stabilized by weak C—H···N hydrogen bonds.

Related literature

For a related structure, see: Wang *et al.* (2007). For background to the use of flexible ligands to form coordination networks, see: Martin *et al.* (2007); Yaghi *et al.* (1998); Sun *et al.* (2006).



Experimental

Crystal data

$C_{18}H_{16}N_6$
M_r = 316.37
Monoclinic, $P2_1/c$
a = 16.590 (3) Å
b = 5.3646 (9) Å
c = 8.8009 (14) Å
β = 92.567 (3)°
V = 782.5 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 298 K
0.21 × 0.17 × 0.11 mm

Data collection

Bruker APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.982, T_{max} = 0.991
3679 measured reflections
1402 independent reflections
870 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.107
S = 0.83
1402 reflections
109 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.12 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
C2—H2···N1^{i}	0.93	2.56	3.381 (2)	148

Symmetry code: (i) $-x+1, y+\frac{1}{2}, -z+\frac{3}{2}$.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5117).

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supporting information

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4,4′-Bis(1,2,4-triazol-1-ylmethyl)biphenyl

Jianjun Xu

S1. Comment

It is well-known that those ligands containing a flexible backbone provide a bigger number of complexes thanks to their flexibility and conformational freedom that allow for greater structural diversity (Yaghi *et al.*, 1998; Sun *et al.*, 2006; Martin *et al.*, 2007).

4,4′-Bis(1,2,4-triazol-1-ylmethyl)biphenyl (bix) is a excellent building block and has been employed to construct interesting structural polymer with unique properties (Wang *et al.*, 2007).

In an attempt to form a Zn(II) complex with bix, we adventitiously formed the title compound (I) and its crystal structure is determined herein.

The title compound cyrstallizes with one half-molecule in the asymmetric unit. As illustrated in Fig. 1, the bix adopts a anti conformation and has crystallographic $\bar{1}$ symmetry and the dihedral angle between the benzene and triazole rings is 84.1 (3)°.

In the crystal structure, weak intermolecular C—H···N hydrogen bond help to stabilizing the packing.

S2. Experimental

Equimolar (28 mg, 0.1 mmol) $Zn(OAC)_2.6H_2O$ in water (3 ml) and bix (26 mg, 0.1 mmol) in CH_3CN and CH3OH solutions (8 ml) were mixed and heated at 428 K for 72 h in a pressurized reactor. Slow evaporation of this solution resulted in the formation of some colourless blocks of (I).

S3. Refinement

All H atoms were fixed geometrically and treated as riding with C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$.

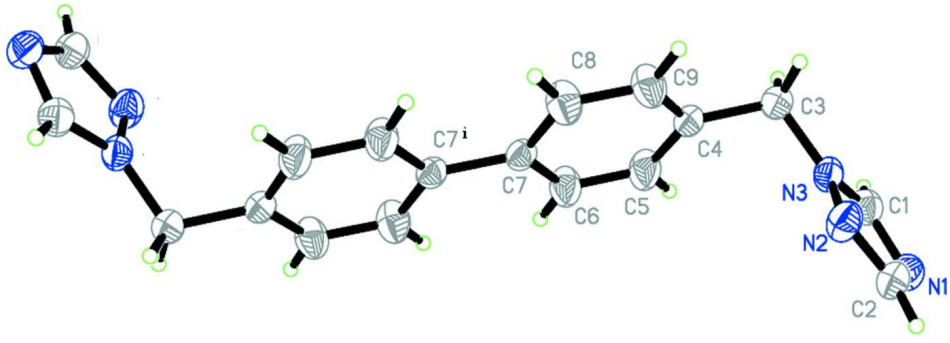

Figure 1

View of (I), showing ellipsoids drawn at the the 30% probability level. H atoms are shown as spheres of arbitrary radius. Symmetry code: (i) –x, 1–y, 1–z.

4,4′-Bis(1,2,4-triazol-1-ylmethyl)biphenyl

Crystal data

$C_{18}H_{16}N_6$
$M_r = 316.37$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 16.590$ (3) Å
$b = 5.3646$ (9) Å
$c = 8.8009$ (14) Å
$\beta = 92.567$ (3)°
$V = 782.5$ (2) Å^3
$Z = 2$
$F(000) = 332$
$D_x = 1.343$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1402 reflections
$\theta = 2.5$–25.2°
$\mu = 0.09$ mm^{-1}
$T = 298$ K
Block, colourless
0.21 × 0.17 × 0.11 mm

Data collection

Bruker APEXII area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min} = 0.982$, $T_{max} = 0.991$
3679 measured reflections
1402 independent reflections
870 reflections with $I > 2\sigma(I)$
$R_{int} = 0.023$
$\theta_{max} = 25.2°$, $\theta_{min} = 2.5°$
$h = -19 \rightarrow 18$
$k = -6 \rightarrow 5$
$l = -10 \rightarrow 10$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.107$
$S = 0.83$
1402 reflections
109 parameters
0 restraints
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
$w = 1/[\sigma^2(F_o^2) + (0.05P)^2 + 0.3476P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.12$ e Å^{-3}
$\Delta\rho_{min} = -0.13$ e Å^{-3}

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.

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}
N3	0.34746 (8)	0.4361 (3)	0.45637 (17)	0.0522 (4)
C7	0.04239 (10)	0.4897 (3)	0.4755 (2)	0.0465 (5)
C4	0.20243 (10)	0.4473 (4)	0.3827 (2)	0.0511 (5)
C3	0.28751 (10)	0.4191 (4)	0.3315 (2)	0.0602 (6)

H3A	0.2927	0.2590	0.2817	0.072*
H3B	0.2979	0.5479	0.2576	0.072*
N2	0.35680 (10)	0.6499 (3)	0.5390 (2)	0.0651 (5)
C2	0.41506 (12)	0.5892 (5)	0.6378 (2)	0.0656 (6)
H2	0.4352	0.7001	0.7113	0.079*
N1	0.44371 (10)	0.3558 (4)	0.6256 (2)	0.0680 (5)
C6	0.09257 (11)	0.2995 (5)	0.5269 (3)	0.0714 (7)
H6	0.0733	0.1827	0.5945	0.086*
C1	0.39952 (12)	0.2674 (4)	0.5101 (2)	0.0605 (6)
H1	0.4042	0.1071	0.4713	0.073*
C9	0.15350 (12)	0.6357 (4)	0.3306 (3)	0.0673 (6)
H9	0.1732	0.7527	0.2638	0.081*
C8	0.07478 (12)	0.6559 (4)	0.3758 (3)	0.0682 (6)
H8	0.0428	0.7858	0.3374	0.082*
C5	0.17066 (11)	0.2789 (5)	0.4804 (3)	0.0718 (7)
H5	0.2025	0.1471	0.5165	0.086*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N3	0.0403 (8)	0.0588 (10)	0.0573 (9)	−0.0008 (8)	0.0015 (7)	−0.0034 (8)
C7	0.0429 (9)	0.0495 (11)	0.0467 (10)	−0.0041 (8)	−0.0038 (8)	−0.0044 (9)
C4	0.0423 (10)	0.0637 (13)	0.0470 (10)	−0.0044 (9)	−0.0030 (8)	−0.0056 (10)
C3	0.0468 (11)	0.0801 (15)	0.0535 (11)	−0.0024 (10)	0.0002 (9)	−0.0071 (11)
N2	0.0543 (10)	0.0649 (12)	0.0754 (12)	−0.0021 (9)	−0.0055 (8)	−0.0133 (10)
C2	0.0507 (11)	0.0816 (17)	0.0640 (13)	−0.0115 (12)	−0.0022 (10)	−0.0072 (12)
N1	0.0562 (10)	0.0846 (14)	0.0627 (11)	0.0017 (10)	−0.0025 (8)	0.0150 (10)
C6	0.0494 (12)	0.0846 (17)	0.0804 (15)	0.0065 (11)	0.0063 (10)	0.0323 (13)
C1	0.0572 (12)	0.0605 (13)	0.0640 (13)	0.0020 (10)	0.0057 (10)	0.0072 (11)
C9	0.0586 (12)	0.0620 (14)	0.0826 (15)	0.0013 (11)	0.0168 (11)	0.0155 (12)
C8	0.0592 (13)	0.0582 (13)	0.0880 (16)	0.0095 (11)	0.0140 (11)	0.0177 (12)
C5	0.0474 (12)	0.0834 (17)	0.0843 (16)	0.0113 (11)	0.0012 (10)	0.0264 (13)

Geometric parameters (Å, º)

N3—C1	1.324 (2)	N2—C2	1.312 (3)
N3—N2	1.363 (2)	C2—N1	1.345 (3)
N3—C3	1.451 (2)	C2—H2	0.9300
C7—C8	1.377 (3)	N1—C1	1.315 (3)
C7—C6	1.380 (3)	C6—C5	1.380 (3)
C7—C7^{i}	1.494 (3)	C6—H6	0.9300
C4—C9	1.363 (3)	C1—H1	0.9300
C4—C5	1.369 (3)	C9—C8	1.386 (3)
C4—C3	1.508 (3)	C9—H9	0.9300
C3—H3A	0.9700	C8—H8	0.9300
C3—H3B	0.9700	C5—H5	0.9300
C1—N3—N2	109.13 (15)	N1—C2—H2	122.3

C1—N3—C3	129.93 (18)	C1—N1—C2	102.16 (18)
N2—N3—C3	120.94 (16)	C7—C6—C5	121.5 (2)
C8—C7—C6	116.16 (17)	C7—C6—H6	119.3
C8—C7—C7^{i}	122.4 (2)	C5—C6—H6	119.3
C6—C7—C7^{i}	121.5 (2)	N1—C1—N3	111.2 (2)
C9—C4—C5	117.42 (18)	N1—C1—H1	124.4
C9—C4—C3	121.69 (19)	N3—C1—H1	124.4
C5—C4—C3	120.87 (19)	C4—C9—C8	121.1 (2)
N3—C3—C4	112.74 (15)	C4—C9—H9	119.5
N3—C3—H3A	109.0	C8—C9—H9	119.5
C4—C3—H3A	109.0	C7—C8—C9	122.1 (2)
N3—C3—H3B	109.0	C7—C8—H8	118.9
C4—C3—H3B	109.0	C9—C8—H8	118.9
H3A—C3—H3B	107.8	C4—C5—C6	121.7 (2)
C2—N2—N3	101.99 (17)	C4—C5—H5	119.1
N2—C2—N1	115.49 (19)	C6—C5—H5	119.1
N2—C2—H2	122.3		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···N1^{ii}	0.93	2.56	3.381 (2)	148

Symmetry code: (ii) $-x$+1, y+1/2, $-z$+3/2.