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4,4′-Bis(benzimidazol-1-yl)biphenyl

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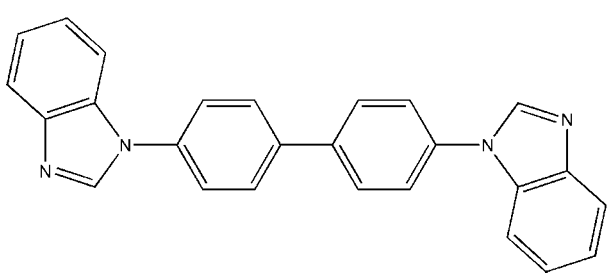
Key indicators: single-crystal X-ray study; *T* = 293 K; mean σ(C–C) = 0.002 Å; *R* factor = 0.036; *wR* factor = 0.103; data-to-parameter ratio = 12.0.

The molecule of the title compound, $C_{26}H_{18}N_4$, resides on a crystallographic inversion centre with a dihedral angle of 44.94 (5)° between the benzimidazole ring system and the benzene ring. The primary hydrogen bond is C—H···N and inversion-related pairs of these generate a chain of rings along the *c*-axis direction; π···π stacking involving the benzimidazole groups with interplanar separations of *ca* 3.4 Å complete the interactions.

Related literature

For related literature, see: Bu *et al.* (2007); Buchwald *et al.* (2001); Cristau *et al.* (2004); Su *et al.* (2003).



Experimental

Crystal data

$C_{26}H_{18}N_4$
M_r = 386.44
Monoclinic, *C*2/*c*
a = 19.628 (4) Å
b = 6.8964 (14) Å
c = 13.760 (3) Å
β = 90.74 (3)°
V = 1862.4 (7) Å^3
Z = 4
Mo *K*α radiation
μ = 0.08 mm^{-1}
T = 293 (2) K
0.26 × 0.22 × 0.10 mm

Data collection

Bruker SMART 1000 CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
T_{min} = 0.904, T_{max} = 1.000 (expected range = 0.897–0.992)
9091 measured reflections
1644 independent reflections
1415 reflections with $I > 2\sigma(I)$
R_{int} = 0.037

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.103
S = 1.10
1644 reflections
137 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C6—H6···N1^{i}	0.93	2.61	3.425 (2)	147

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GG2046).

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supplementary materials

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4,4'-Bis(benzimidazol-1-yl)biphenyl

Z.-X. Li, Y. Zuo and T.-L. Hu

Comment

In recent years, benzimidazole derivatives have been found a wide range of application in the area of coordination chemistry, because they exhibit a strong networking ability (Bu *et al.*, 2007; Su *et al.*, 2003). The title compound has been designed for building polymer architectures. We report here the structure and conformation, towards an understanding of the ligand coordination. As shown in Fig. 1, the title compound has *trans*-conformation and therefore a tendency to *trans*-coordination. The molecule resides on an inversion centre, and the dihedral angle between the benzimidazole ring and the phenyl ring is 40.97 (17)°. There are weak H-bonding interactions in the crystal structure of (I) (C6—H6···N1B, 3.425 (17) Å, C—H···N of 146.82 (13)°, B= *x*,-*y* + 2,*z* + 1/2) (Fig. 2).

Experimental

The ligand 4,4'-di(benzimidazol-1-yl)biphenyl was prepared by a modified method (Buchwald *et al.*, 2001; Cristau *et al.*, 2004). A mixture of 4,4'-dibromobiphenyl (3.75 g, 12.0 mmol), benzimidazole (7.08 g, 60.0 mmol), CuI (0.47 g, 2.5 mmol), 1,10-phenanthroline (1.19 g, 6.0 mmol), and K_2CO_3 (13.27 g, 96.0 mmol) was suspended in DMF (120 ml) and refluxed for 4 days to afford (I) as light-yellow powder, yield: 30% (based on 4,4'-dibromobiphenyl). *M*.p.: 566 K. MS (ESI): m/*z*=387.45. Anal calcd for $C_{26}H_{18}N_4$: C, 80.81%; H, 4.69%; N, 14.50%. Found: C, 80.56%; H, 4.48%; N, 14.31%. Single crystals were obtained by recrystallizing from a mixture of $CHCl_3$ and CH_3OH (1:1).

Refinement

C-bound H atoms were positioned geometrically and refined in the riding-model approximation, with C—H = 0.93Å and U_{iso}(H) = 1.2U_{eq}.

Figures

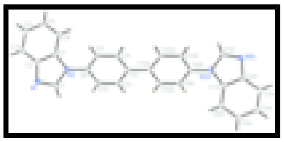


Fig. 1. The molecular structure of (I). Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radius [symmetry code: (A) −*x* + 1,-*y* + 2,-*z* + 1].

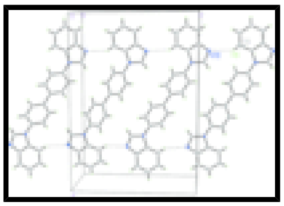


Fig. 2. The crystal packing for (I) [symmetry code: (B) *x*,-*y* + 2,*z* + 1/2].

4,4'-Bis(benzimidazol-1-yl)biphenyl

Crystal data

$C_{26}H_{18}N_4$	F_{000} = 808
M_r = 386.44	D_x = 1.378 Mg m^{-3}
Monoclinic, $C2/c$	Melting point: 566 K
Hall symbol: -c 2yc	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 19.628 (4) Å	Cell parameters from 2932 reflections
b = 6.8964 (14) Å	θ = 2.6–28.7º
c = 13.760 (3) Å	μ = 0.08 mm^{-1}
β = 90.74 (3)º	T = 293 (2) K
V = 1862.4 (7) Å^3	Block, colorless
Z = 4	0.26 × 0.22 × 0.10 mm

Data collection

Bruker SMART 1000 CCD diffractometer	1644 independent reflections
Radiation source: fine-focus sealed tube	1415 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.037
Detector resolution: 9 pixels mm^{-1}	θ_{max} = 25.0º
T = 293(2) K	θ_{min} = 3.0º
ω scans	$h = -23 \rightarrow 23$
Absorption correction: multi-scan (SADABS; Bruker, 1998)	$k = -8 \rightarrow 8$
T_{min} = 0.904, T_{max} = 1.000	$l = -16 \rightarrow 16$
9091 measured reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.037	$w = 1/[\sigma^2(F_o^2) + (0.0718P)^2 + 0.0391P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.103	$(\Delta/\sigma)_{max}$ = 0.001
S = 1.10	$\Delta\rho_{max}$ = 0.18 e Å^{-3}
1644 reflections	$\Delta\rho_{min}$ = −0.17 e Å^{-3}
137 parameters	Extinction correction: SHELXL, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.032 (4)
Secondary atom site location: difference Fourier map	

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 $F^2 > 2\text{sigma}(F^2)$ 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}
N1	0.22326 (5)	0.98108 (14)	0.82891 (7)	0.0259 (3)
N2	0.28767 (5)	0.99037 (13)	0.69471 (7)	0.0196 (3)
C1	0.28458 (6)	0.99959 (16)	0.79430 (8)	0.0233 (3)
H1	0.3229	1.0175	0.8337	0.028*
C2	0.18197 (6)	0.95587 (16)	0.74690 (8)	0.0217 (3)
C3	0.11196 (6)	0.91962 (17)	0.74020 (9)	0.0271 (3)
H3	0.0854	0.9134	0.7956	0.033*
C4	0.08336 (6)	0.89337 (17)	0.64895 (9)	0.0289 (4)
H4	0.0369	0.8694	0.6429	0.035*
C5	0.12330 (6)	0.90221 (16)	0.56532 (9)	0.0269 (3)
H5	0.1025	0.8845	0.5049	0.032*
C6	0.19250 (6)	0.93632 (16)	0.56982 (8)	0.0221 (3)
H6	0.2189	0.9410	0.5142	0.027*
C7	0.22077 (6)	0.96335 (15)	0.66211 (9)	0.0197 (3)
C8	0.34804 (6)	0.99569 (15)	0.63884 (8)	0.0191 (3)
C9	0.35123 (6)	1.10302 (16)	0.55419 (8)	0.0239 (3)
H9	0.3136	1.1741	0.5331	0.029*
C10	0.41052 (6)	1.10460 (16)	0.50080 (9)	0.0234 (3)
H10	0.4118	1.1770	0.4438	0.028*
C11	0.46851 (6)	1.00092 (15)	0.52969 (8)	0.0195 (3)
C12	0.46409 (6)	0.89818 (18)	0.61685 (8)	0.0268 (3)
H12	0.5021	0.8305	0.6396	0.032*
C13	0.40515 (6)	0.89417 (18)	0.67017 (8)	0.0256 (3)
H13	0.4037	0.8229	0.7275	0.031*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0289 (6)	0.0284 (6)	0.0204 (6)	−0.0051 (4)	0.0060 (5)	−0.0016 (4)
N2	0.0212 (6)	0.0207 (5)	0.0170 (6)	−0.0025 (4)	0.0038 (4)	−0.0006 (4)
C1	0.0271 (7)	0.0255 (6)	0.0172 (7)	−0.0033 (5)	0.0019 (5)	−0.0006 (5)
C2	0.0255 (6)	0.0185 (6)	0.0211 (7)	−0.0009 (5)	0.0058 (5)	−0.0011 (5)

C3	0.0249 (7)	0.0249 (7)	0.0318 (8)	−0.0006 (5)	0.0103 (5)	−0.0007 (5)
C4	0.0213 (6)	0.0244 (7)	0.0409 (8)	−0.0001 (5)	0.0012 (6)	0.0000 (5)
C5	0.0279 (7)	0.0235 (7)	0.0292 (7)	0.0013 (5)	−0.0044 (5)	−0.0002 (5)
C6	0.0267 (6)	0.0191 (6)	0.0206 (7)	0.0014 (5)	0.0015 (5)	0.0008 (5)
C7	0.0212 (6)	0.0155 (6)	0.0226 (7)	−0.0004 (4)	0.0025 (5)	0.0011 (4)
C8	0.0203 (6)	0.0191 (6)	0.0178 (6)	−0.0045 (4)	0.0034 (5)	−0.0033 (4)
C9	0.0256 (6)	0.0217 (7)	0.0245 (7)	0.0049 (5)	0.0046 (5)	0.0031 (5)
C10	0.0298 (7)	0.0203 (6)	0.0203 (6)	0.0009 (5)	0.0059 (5)	0.0037 (5)
C11	0.0196 (7)	0.0204 (6)	0.0185 (7)	−0.0070 (4)	0.0003 (5)	−0.0025 (4)
C12	0.0166 (6)	0.0412 (8)	0.0227 (7)	−0.0021 (5)	−0.0016 (5)	0.0071 (5)
C13	0.0218 (6)	0.0369 (7)	0.0181 (7)	−0.0055 (5)	−0.0012 (5)	0.0078 (5)

Geometric parameters (Å, °)

C9—C8	1.3822 (16)	C5—C6	1.3790 (17)
C9—C10	1.3842 (16)	C5—C4	1.4021 (18)
C9—H9	0.9300	C5—H5	0.9300
N2—C1	1.3740 (15)	C4—C3	1.3806 (18)
N2—C7	1.3945 (15)	C4—H4	0.9300
N2—C8	1.4212 (15)	C13—C12	1.3781 (16)
C10—C11	1.3974 (17)	C13—C8	1.3856 (17)
C10—H10	0.9300	C13—H13	0.9300
N1—C1	1.3063 (16)	C12—H12	0.9300
N1—C2	1.3916 (16)	C2—C3	1.3986 (17)
C11—C12	1.3967 (17)	C3—H3	0.9300
C11—C11^{i}	1.491 (2)	C6—H6	0.9300
C7—C6	1.3918 (17)	C1—H1	0.9300
C7—C2	1.4024 (17)		
C8—C9—C10	119.93 (11)	C12—C13—C8	120.37 (11)
C8—C9—H9	120.0	C12—C13—H13	119.8
C10—C9—H9	120.0	C8—C13—H13	119.8
C1—N2—C7	105.87 (10)	C13—C12—C11	121.94 (11)
C1—N2—C8	125.89 (11)	C13—C12—H12	119.0
C7—N2—C8	128.14 (10)	C11—C12—H12	119.0
C9—C10—C11	122.16 (11)	N1—C2—C3	129.57 (11)
C9—C10—H10	118.9	N1—C2—C7	110.69 (10)
C11—C10—H10	118.9	C3—C2—C7	119.70 (11)
C1—N1—C2	104.25 (10)	C4—C3—C2	118.10 (12)
C12—C11—C10	116.39 (11)	C4—C3—H3	120.9
C12—C11—C11^{i}	121.83 (13)	C2—C3—H3	120.9
C10—C11—C11^{i}	121.78 (13)	C9—C8—C13	119.18 (11)
C6—C7—N2	132.38 (11)	C9—C8—N2	121.11 (10)
C6—C7—C2	122.66 (11)	C13—C8—N2	119.70 (11)
N2—C7—C2	104.86 (10)	C5—C6—C7	116.40 (11)
C6—C5—C4	122.10 (12)	C5—C6—H6	121.8
C6—C5—H5	118.9	C7—C6—H6	121.8
C4—C5—H5	118.9	N1—C1—N2	114.33 (12)
C3—C4—C5	121.03 (11)	N1—C1—H1	122.8

C3—C4—H4	119.5	N2—C1—H1	122.8
C5—C4—H4	119.5		
C8—C9—C10—C11	−0.30 (18)	C5—C4—C3—C2	0.17 (17)
C9—C10—C11—C12	−1.33 (17)	N1—C2—C3—C4	−177.73 (11)
C9—C10—C11—C11^{i}	178.27 (12)	C7—C2—C3—C4	−0.38 (16)
C1—N2—C7—C6	−177.15 (12)	C10—C9—C8—C13	1.41 (16)
C8—N2—C7—C6	−0.74 (18)	C10—C9—C8—N2	−179.55 (10)
C1—N2—C7—C2	−0.74 (11)	C12—C13—C8—C9	−0.85 (17)
C8—N2—C7—C2	175.68 (10)	C12—C13—C8—N2	−179.90 (10)
C6—C5—C4—C3	0.30 (18)	C1—N2—C8—C9	−138.05 (12)
C8—C13—C12—C11	−0.85 (18)	C7—N2—C8—C9	46.20 (15)
C10—C11—C12—C13	1.90 (17)	C1—N2—C8—C13	40.98 (16)
C11^{i}—C11—C12—C13	−177.70 (12)	C7—N2—C8—C13	−134.76 (12)
C1—N1—C2—C3	176.54 (12)	C4—C5—C6—C7	−0.53 (17)
C1—N1—C2—C7	−1.00 (12)	N2—C7—C6—C5	176.21 (11)
C6—C7—C2—N1	177.95 (10)	C2—C7—C6—C5	0.32 (16)
N2—C7—C2—N1	1.09 (12)	C2—N1—C1—N2	0.52 (13)
C6—C7—C2—C3	0.13 (17)	C7—N2—C1—N1	0.14 (13)
N2—C7—C2—C3	−176.73 (10)	C8—N2—C1—N1	−176.38 (9)

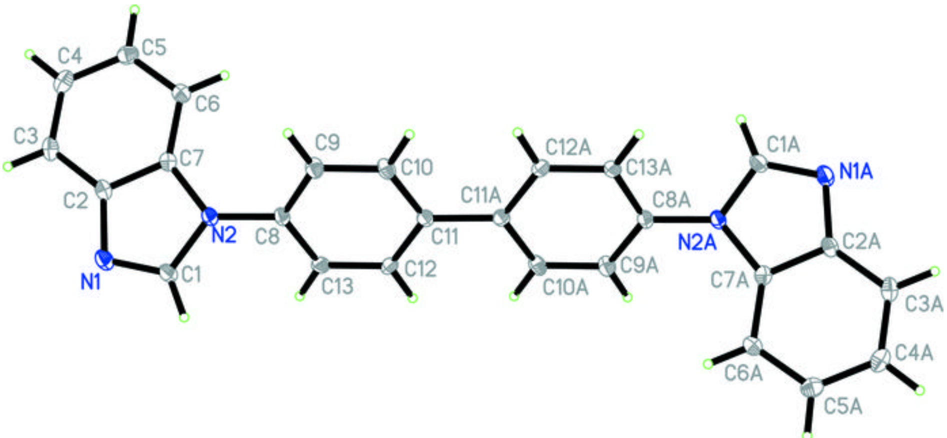
Symmetry codes: (i) $-x+1, -y+2, -z+1$.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C6—H6···N1^{ii}	0.93	2.61	3.425 (2)	147

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

Fig. 1


C4
C5
C6
C3
C7
C9
C10
C12A
C13A
C1A
N1A
C2
N2
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C11A
C11
C8A
N2A
C2A
N1
C1
C13
C12
C10A
C9A
C7A
C3A
C6A
C4A
C5A

Fig. 2