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1,4-Bis(1*H*-benzimidazol-1-yl)benzene

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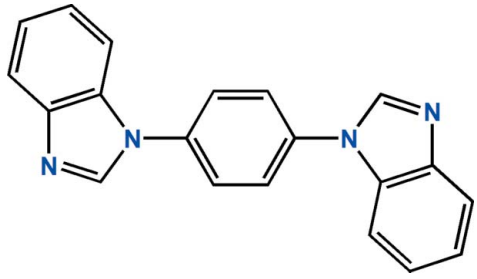
Key indicators: single-crystal X-ray study; T = 293 K, P = 0.0 kPa; mean σ(C–C) = 0.005 Å; R factor = 0.051; wR factor = 0.104; data-to-parameter ratio = 6.4.

In the title compound, $C_{20}H_{14}N_4$, the dihedral angles between the central benzene ring and the pendant benzimidazole ring systems are 46.60 (15) and 47.89 (16)°. The dihedral angle between the benzimidazole ring systems is 85.62 (12)° and the N atoms lie to the same side of the molecule. In the crystal, molecules are linked by C—H···N interactions and weak aromatic π–π stacking [shortest centroid–centroid separation = 3.770 (2) Å] is observed.

Related literature

For background to benzimidazole derivatives as ligands in crystal engineering, see: Li *et al.* (2009); Vijayan *et al.* (2006).



Experimental

Crystal data

$C_{20}H_{14}N_4$ M_r = 310.35
Orthorhombic, $Pna2_1$
a = 9.5458 (19) Å
b = 20.499 (4) Å
c = 7.9283 (16) Å
V = 1551.4 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 293 K
0.25 × 0.22 × 0.18 mm

Data collection

Rigaku Mercury CCD diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2005)
T_{min} = 0.980, T_{max} = 0.985
12744 measured reflections
1479 independent reflections
1298 reflections with $I > 2\sigma(I)$
R_{int} = 0.075

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.104
S = 1.17
1479 reflections
231 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1···N4^{i}	0.93	2.50	3.359 (5)	153
C6—H6···N4^{ii}	0.93	2.56	3.447 (5)	159

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

Data collection: *CrystalClear* (Rigaku/MSC, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB6340).

References

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Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Vijayan, N., Bhagavannarayana, G., Balamurugan, N., Babu, R. R., Maurya, K. K., Gopalakrishnan, R. & Ramasamy, P. (2006). *J. Cryst. Growth*, **293**, 318–323.

supplementary materials

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1,4-Bis(1*H*-benzimidazol-1-yl)benzene

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Comment

In recent years, benzimidazole has been well used in crystal engineering, because they exhibit a strong networking ability (Vijayan *et al.*, 2006). To our knowledge, the research on benzimidazole ligands bearing rigid spacers is still less developed (Li *et al.*, 2009), and the title compound was well designed for building polymer architecture. We report here the structure and conformation of a rigid benzimidazole derivative, and further explore the ligand coordination. As shown in Fig. 1, the title compound is *trans*-conformation and tends to *trans*-coordination. The molecule has no inversion centre because two benzimidazole rings are not coplanar.

Experimental

The ligand 1,4-di(1*H*-benzimidazol-1-yl)benzene was prepared by a modified method (Li *et al.*, 2009). A mixture of 1,4-dibromophenyl (3.72 g, 12.0 mmol), benzimidazole (4.25 g, 36.0 mmol), CuI (0.38 g, 2.0 mmol), 1,10-phenanthroline (0.72 g, 4.0 mmol), and Cs_2CO_3 (2.48 g, 18.0 mmol) was suspended in DMF (50 ml) and refluxed for 48 h to afford (I) as off-white powder, yield: 25% (based on 1,4-dibromophenyl), Mp: 291°C. Colourless blocks of (I) were obtained by recrystallizing from a mixed solvent of methanol and water (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}. Anomalous dispersion was negligible and Friedel pairs were merged before refinement.

Figures

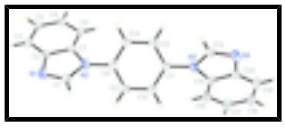

Fig. 1. The molecular structure of (I). Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radius.

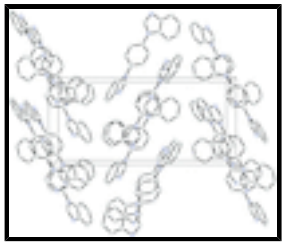

Fig. 2. The crystal packing for (I).

1,4-Bis(1*H*-benzimidazol-1-yl)benzene

Crystal data

$C_{20}H_{14}N_4$	$D_x = 1.329$ Mg m^{-3}
$M_r = 310.35$	Melting point: 564 K
Orthorhombic, $Pna2_1$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: P 2c -2n	Cell parameters from 13068 reflections
$a = 9.5458$ (19) Å	$\theta = 3.3$–$27.6°$
$b = 20.499$ (4) Å	$\mu = 0.08$ mm^{-1}
$c = 7.9283$ (16) Å	$T = 293$ K
$V = 1551.4$ (5) Å^3	Block, colorless
$Z = 4$	0.25 × 0.22 × 0.18 mm
$F(000) = 648$	

Data collection

Rigaku Mercury CCD diffractometer	1479 independent reflections
Radiation source: fine-focus sealed tube	1298 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.075$
Detector resolution: 9 pixels mm^{-1}	$\theta_{max} = 25.0°$, $\theta_{min} = 3.5°$
ω scans	$h = -11 \rightarrow 11$
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2005)	$k = -24 \rightarrow 24$
$T_{min} = 0.980$, $T_{max} = 0.985$	$l = -9 \rightarrow 9$
12744 measured reflections	

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.051$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.104$	H-atom parameters constrained
$S = 1.17$	$w = 1/[\sigma^2(F_o^2) + (0.0488P)^2 + 0.1271P]$ where $P = (F_o^2 + 2F_c^2)/3$
1479 reflections	$(\Delta/\sigma)_{max} < 0.001$
231 parameters	$\Delta\rho_{max} = 0.14$ e Å^{-3}
1 restraint	$\Delta\rho_{min} = -0.16$ e Å^{-3}
0 constraints	

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_{iso}*/U_{eq}
N1	0.2140 (3)	0.55131 (15)	0.6320 (4)	0.0462 (8)
N2	0.4461 (3)	0.53457 (14)	0.6010 (4)	0.0411 (8)
N3	0.9643 (3)	0.40659 (14)	0.6681 (4)	0.0383 (7)
N4	1.1632 (3)	0.37523 (15)	0.7980 (4)	0.0479 (9)
C1	0.3178 (4)	0.51125 (18)	0.6527 (5)	0.0452 (9)
H1	0.3065	0.4699	0.6993	0.043 (10)*
C2	0.2750 (3)	0.60700 (16)	0.5602 (4)	0.0361 (8)
C3	0.2141 (4)	0.66544 (17)	0.5108 (5)	0.0427 (9)
H3	0.1189	0.6729	0.5263	0.036 (9)*
C4	0.2986 (4)	0.71179 (17)	0.4385 (5)	0.0421 (9)
H4	0.2598	0.7513	0.4047	0.063 (13)*
C5	0.4412 (4)	0.70086 (17)	0.4146 (5)	0.0442 (10)
H5	0.4948	0.7331	0.3629	0.046 (11)*
C6	0.5059 (4)	0.64388 (17)	0.4649 (5)	0.0431 (9)
H6	0.6014	0.6371	0.4499	0.045 (10)*
C7	0.4197 (3)	0.59693 (16)	0.5399 (5)	0.0364 (8)
C8	0.5788 (3)	0.50222 (17)	0.6151 (4)	0.0379 (9)
C9	0.5905 (4)	0.43768 (17)	0.5667 (5)	0.0419 (9)
H9	0.5134	0.4158	0.5226	0.058 (12)*
C10	0.7177 (3)	0.40549 (17)	0.5842 (5)	0.0408 (9)
H10	0.7256	0.3618	0.5539	0.037 (9)*
C11	0.8327 (3)	0.43899 (17)	0.6469 (5)	0.0366 (8)
C12	0.8204 (4)	0.50358 (17)	0.6927 (5)	0.0421 (9)
H12	0.8982	0.5260	0.7330	0.047 (11)*
C13	0.6930 (4)	0.53532 (18)	0.6794 (5)	0.0455 (10)
H13	0.6843	0.5786	0.7130	0.037 (10)*
C14	1.0470 (4)	0.40901 (19)	0.8087 (5)	0.0443 (9)
H14	1.0229	0.4329	0.9042	0.046 (11)*
C15	1.0353 (3)	0.36720 (16)	0.5527 (5)	0.0391 (9)
C16	1.0063 (4)	0.3484 (2)	0.3891 (6)	0.0523 (11)
H16	0.9241	0.3610	0.3355	0.064 (13)*
C17	1.1043 (4)	0.3103 (2)	0.3088 (6)	0.0662 (12)
H17	1.0880	0.2971	0.1983	0.086 (16)*

C18	1.2279 (5)	0.2907 (2)	0.3899 (6)	0.0650 (13)
H18	1.2914	0.2644	0.3325	0.055 (12)*
C19	1.2571 (4)	0.30983 (19)	0.5533 (6)	0.0525 (10)
H19	1.3397	0.2973	0.6065	0.065 (13)*
C20	1.1584 (4)	0.34847 (17)	0.6357 (5)	0.0423 (9)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0327 (17)	0.0505 (18)	0.056 (2)	0.0003 (15)	0.0048 (16)	0.0058 (17)
N2	0.0318 (16)	0.0426 (18)	0.049 (2)	0.0027 (13)	0.0035 (15)	0.0057 (15)
N3	0.0292 (15)	0.0410 (16)	0.0448 (18)	0.0019 (13)	−0.0052 (14)	0.0046 (16)
N4	0.040 (2)	0.058 (2)	0.046 (2)	0.0025 (16)	−0.0089 (16)	0.0052 (18)
C1	0.041 (2)	0.038 (2)	0.057 (2)	−0.0039 (17)	0.010 (2)	0.009 (2)
C2	0.0285 (17)	0.0417 (19)	0.038 (2)	−0.0029 (16)	0.0033 (17)	−0.0012 (17)
C3	0.034 (2)	0.047 (2)	0.047 (2)	0.0072 (17)	0.0010 (17)	−0.0050 (19)
C4	0.039 (2)	0.0353 (18)	0.052 (2)	0.0059 (17)	0.0013 (19)	0.0000 (19)
C5	0.044 (2)	0.038 (2)	0.051 (2)	−0.0019 (18)	0.0041 (19)	0.003 (2)
C6	0.031 (2)	0.047 (2)	0.052 (2)	−0.0003 (17)	0.0011 (19)	−0.0041 (19)
C7	0.0305 (18)	0.0354 (19)	0.043 (2)	0.0001 (15)	0.0014 (17)	−0.0035 (19)
C8	0.0363 (19)	0.041 (2)	0.036 (2)	0.0057 (15)	0.0021 (16)	0.0033 (17)
C9	0.0316 (19)	0.042 (2)	0.052 (2)	−0.0021 (16)	−0.0049 (18)	0.0017 (19)
C10	0.039 (2)	0.038 (2)	0.046 (2)	0.0017 (17)	−0.0042 (17)	−0.0015 (18)
C11	0.0318 (19)	0.044 (2)	0.0339 (19)	0.0024 (15)	−0.0022 (17)	0.0042 (18)
C12	0.034 (2)	0.043 (2)	0.049 (2)	−0.0014 (17)	−0.0066 (17)	−0.0030 (19)
C13	0.044 (2)	0.039 (2)	0.054 (3)	0.0039 (17)	−0.0021 (19)	−0.0105 (19)
C14	0.039 (2)	0.053 (2)	0.041 (2)	−0.0013 (19)	−0.0063 (19)	0.001 (2)
C15	0.0338 (19)	0.0346 (18)	0.049 (2)	0.0030 (15)	−0.0013 (18)	0.0040 (18)
C16	0.048 (2)	0.061 (3)	0.048 (2)	0.013 (2)	−0.013 (2)	−0.007 (2)
C17	0.064 (3)	0.079 (3)	0.056 (3)	0.024 (2)	−0.004 (2)	−0.015 (3)
C18	0.057 (3)	0.068 (3)	0.070 (3)	0.024 (2)	0.003 (2)	−0.010 (3)
C19	0.042 (2)	0.056 (2)	0.060 (3)	0.011 (2)	−0.005 (2)	0.006 (2)
C20	0.037 (2)	0.041 (2)	0.049 (2)	0.0012 (16)	−0.0034 (19)	0.005 (2)

Geometric parameters (Å, °)

N1—C1	1.298 (5)	C8—C13	1.381 (5)
N1—C2	1.402 (4)	C8—C9	1.382 (5)
N2—C1	1.377 (4)	C9—C10	1.389 (5)
N2—C7	1.390 (4)	C9—H9	0.9300
N2—C8	1.434 (4)	C10—C11	1.387 (5)
N3—C14	1.367 (4)	C10—H10	0.9301
N3—C15	1.396 (5)	C11—C12	1.378 (5)
N3—C11	1.431 (4)	C12—C13	1.384 (5)
N4—C14	1.310 (4)	C12—H12	0.9299
N4—C20	1.400 (5)	C13—H13	0.9301
C1—H1	0.9301	C14—H14	0.9299
C2—C3	1.388 (5)	C15—C16	1.381 (6)
C2—C7	1.406 (4)	C15—C20	1.400 (5)

C3—C4	1.372 (5)	C16—C17	1.374 (6)
C3—H3	0.9300	C16—H16	0.9299
C4—C5	1.393 (5)	C17—C18	1.402 (6)
C4—H4	0.9299	C17—H17	0.9300
C5—C6	1.380 (5)	C18—C19	1.382 (6)
C5—H5	0.9301	C18—H18	0.9300
C6—C7	1.399 (5)	C19—C20	1.394 (5)
C6—H6	0.9300	C19—H19	0.9301
C1—N1—C2	104.4 (3)	C10—C9—H9	120.0
C1—N2—C7	105.2 (3)	C11—C10—C9	119.5 (3)
C1—N2—C8	127.0 (3)	C11—C10—H10	120.3
C7—N2—C8	127.8 (3)	C9—C10—H10	120.2
C14—N3—C15	106.0 (3)	C12—C11—C10	120.2 (3)
C14—N3—C11	125.8 (3)	C12—C11—N3	119.3 (3)
C15—N3—C11	128.2 (3)	C10—C11—N3	120.5 (3)
C14—N4—C20	103.8 (3)	C11—C12—C13	120.4 (3)
N1—C1—N2	115.0 (3)	C11—C12—H12	119.8
N1—C1—H1	122.5	C13—C12—H12	119.8
N2—C1—H1	122.5	C8—C13—C12	119.4 (3)
C3—C2—N1	130.0 (3)	C8—C13—H13	120.3
C3—C2—C7	120.4 (3)	C12—C13—H13	120.3
N1—C2—C7	109.6 (3)	N4—C14—N3	114.6 (4)
C4—C3—C2	118.0 (3)	N4—C14—H14	122.7
C4—C3—H3	121.0	N3—C14—H14	122.7
C2—C3—H3	120.9	C16—C15—N3	132.8 (3)
C3—C4—C5	121.3 (3)	C16—C15—C20	122.2 (4)
C3—C4—H4	119.3	N3—C15—C20	104.9 (3)
C5—C4—H4	119.4	C17—C16—C15	117.2 (4)
C6—C5—C4	122.3 (4)	C17—C16—H16	121.4
C6—C5—H5	118.9	C15—C16—H16	121.4
C4—C5—H5	118.9	C16—C17—C18	121.5 (5)
C5—C6—C7	116.2 (3)	C16—C17—H17	119.2
C5—C6—H6	121.9	C18—C17—H17	119.3
C7—C6—H6	121.9	C19—C18—C17	121.2 (4)
N2—C7—C6	132.4 (3)	C19—C18—H18	119.4
N2—C7—C2	105.9 (3)	C17—C18—H18	119.4
C6—C7—C2	121.7 (3)	C18—C19—C20	117.7 (4)
C13—C8—C9	120.6 (3)	C18—C19—H19	121.2
C13—C8—N2	119.9 (3)	C20—C19—H19	121.1
C9—C8—N2	119.5 (3)	C19—C20—N4	129.2 (3)
C8—C9—C10	119.8 (3)	C19—C20—C15	120.2 (4)
C8—C9—H9	120.1	N4—C20—C15	110.6 (3)
C2—N1—C1—N2	−0.1 (4)	C14—N3—C11—C12	46.4 (5)
C7—N2—C1—N1	−0.1 (5)	C15—N3—C11—C12	−133.0 (4)
C8—N2—C1—N1	177.2 (4)	C14—N3—C11—C10	−132.3 (4)
C1—N1—C2—C3	179.9 (4)	C15—N3—C11—C10	48.3 (5)
C1—N1—C2—C7	0.2 (4)	C10—C11—C12—C13	1.1 (6)
N1—C2—C3—C4	−178.1 (4)	N3—C11—C12—C13	−177.6 (4)

C7—C2—C3—C4	1.5 (5)	C9—C8—C13—C12	0.9 (6)
C2—C3—C4—C5	0.2 (6)	N2—C8—C13—C12	179.9 (3)
C3—C4—C5—C6	−1.4 (6)	C11—C12—C13—C8	−1.8 (6)
C4—C5—C6—C7	0.8 (6)	C20—N4—C14—N3	0.6 (4)
C1—N2—C7—C6	−177.3 (4)	C15—N3—C14—N4	−0.5 (4)
C8—N2—C7—C6	5.4 (7)	C11—N3—C14—N4	−179.9 (3)
C1—N2—C7—C2	0.2 (4)	C14—N3—C15—C16	−178.0 (4)
C8—N2—C7—C2	−177.1 (3)	C11—N3—C15—C16	1.4 (6)
C5—C6—C7—N2	178.1 (4)	C14—N3—C15—C20	0.1 (4)
C5—C6—C7—C2	1.0 (6)	C11—N3—C15—C20	179.6 (3)
C3—C2—C7—N2	180.0 (3)	N3—C15—C16—C17	177.6 (4)
N1—C2—C7—N2	−0.3 (4)	C20—C15—C16—C17	−0.3 (6)
C3—C2—C7—C6	−2.2 (6)	C15—C16—C17—C18	0.6 (7)
N1—C2—C7—C6	177.6 (4)	C16—C17—C18—C19	−1.0 (7)
C1—N2—C8—C13	−131.9 (4)	C17—C18—C19—C20	1.0 (6)
C7—N2—C8—C13	44.8 (5)	C18—C19—C20—N4	−178.6 (4)
C1—N2—C8—C9	47.1 (5)	C18—C19—C20—C15	−0.6 (5)
C7—N2—C8—C9	−136.2 (4)	C14—N4—C20—C19	177.6 (4)
C13—C8—C9—C10	0.7 (6)	C14—N4—C20—C15	−0.5 (4)
N2—C8—C9—C10	−178.3 (3)	C16—C15—C20—C19	0.3 (5)
C8—C9—C10—C11	−1.4 (6)	N3—C15—C20—C19	−178.1 (3)
C9—C10—C11—C12	0.5 (5)	C16—C15—C20—N4	178.6 (4)
C9—C10—C11—N3	179.2 (3)	N3—C15—C20—N4	0.3 (4)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1···N4^{i}	0.93	2.50	3.359 (5)	153
C6—H6···N4^{ii}	0.93	2.56	3.447 (5)	159

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

Fig. 1

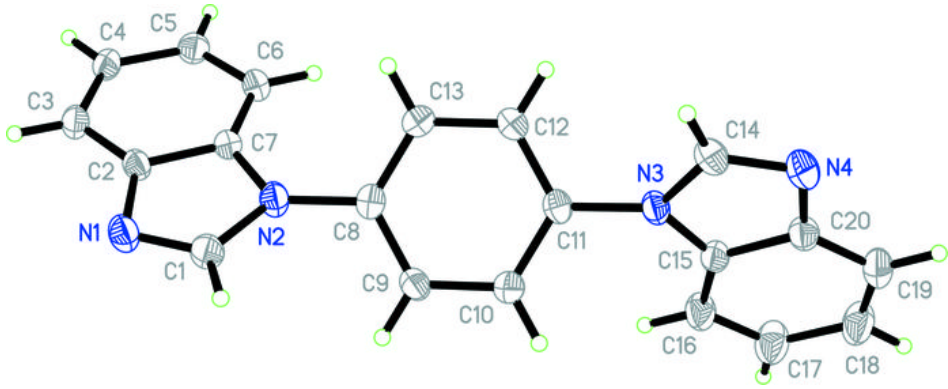
C4
C5
C6
C3
C7
C2
N1
N2
C1
C8
C13
C12
C9
C10
C11
N3
C14
N4
C20
C15
C19
C16
C17
C18

Fig. 2