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2,2′-(Ethane-1,2-diyl)bis(1*H*-benzimidazole)

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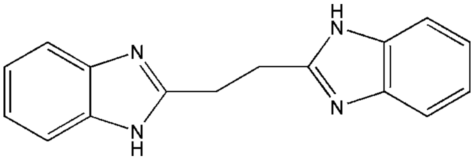
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.002 Å; R factor = 0.045; wR factor = 0.122; data-to-parameter ratio = 16.2.

The complete molecule of the title compound, $C_{16}H_{14}N_4$, is generated by crystallographic inversion symmetry. In the crystal, molecules are linked by N—H⋯N hydrogen bonds, generating (001) sheets. Weak aromatic π–π stacking interactions [centroid–centroid distances = 3.7383 (13) and 3.7935 (14) Å] are also observed.

Related literature

For background to metal-organic frameworks, see: van Albada *et al.* (2007). For the synthesis, see: Wang & Joulli (1957).



Experimental

Crystal data

$C_{16}H_{14}N_4$	M_r = 262.31
Orthorhombic, $Pbca$	Z = 4
a = 8.4295 (18) Å	Mo $K\alpha$ radiation
b = 9.924 (2) Å	μ = 0.08 mm^{-1}
c = 15.351 (4) Å	T = 296 K
V = 1284.2 (5) Å^3	0.32 × 0.25 × 0.19 mm

Data collection

Bruker APEXII CCD diffractometer	10702 measured reflections
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	1475 independent reflections
T_{min} = 0.975, T_{max} = 0.984	966 reflections with $I > 2\sigma(I)$
	R_{int} = 0.052

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045	91 parameters
$wR(F^2)$ = 0.122	H-atom parameters constrained
S = 1.02	$\Delta\rho_{max}$ = 0.15 e Å^{-3}
1475 reflections	$\Delta\rho_{min}$ = −0.21 e Å^{-3}

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

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
N2—H2B⋯N1^{i}	0.86	2.04	2.8568 (18)	159

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

Data collection: *APEX2* (Bruker, 2006); cell refinement: *SAINT* (Bruker, 2006); data reduction: *SAINT*; 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: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB6688).

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supporting information

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2,2′-(Ethane-1,2-diyl)bis(1*H*-benzimidazole)

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S1. Comment

We present a polyaromatic compoud (1) that contains multiple functional groups that can develop a series of metal-organic frameworks with potential applications (e.g. van Albada *et al.* (2007)). The molecular struture of (1), shown in Fig.1, consists of two symmetrical benzimidazole rings. The two benzimidazolyl rings are nearly parallel, witha dihedral angle of 2.645 (6)° between them. Molecules are linked *via* a network of hydrogen bonds (N2—H2B···N1; Table 2). *π*–*π* stacking interactions are observed between nearly parallel benzimidazolyl benzene rings. The centroid-to-centroid distance between C1—C6 benzene rings is 3.7379 Å, while between C1A—C6A benzene rings it is 3.7944 Å (the symmetry operation: -*x* + 1,-*y*,-*z*). The hydrogen bonds and *π*–*π* weak non-covalent interactions lend stability to the structure. The stacking plot of this compound was shown in Fig. 2.

S2. Experimental

o-Phenylenediamine (1.081 g, 10 mmol) and succinic acid (0.590 g, 5 mmol) were refluxed for 4 h in 30 ml of 10% hydrochloric acid solution. The reaction mixture was cooled to room temperature, the precipitation that formed was filtered and then recrystallized from water. The colourless crystals were obtained from water after a week (Wang *et al.*, 1957).

S3. Refinement

The H atoms bonded to C and N atoms were positioned geometrically and refined using a riding model [aliphatic C—H =0.96 Å ($U_{\rm iso}$(H) = 1.5$U_{\rm eq}$(C)), aromatic C—H = 0.93 Å ($U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C)) and N—H = 0.86 Å with $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(N).

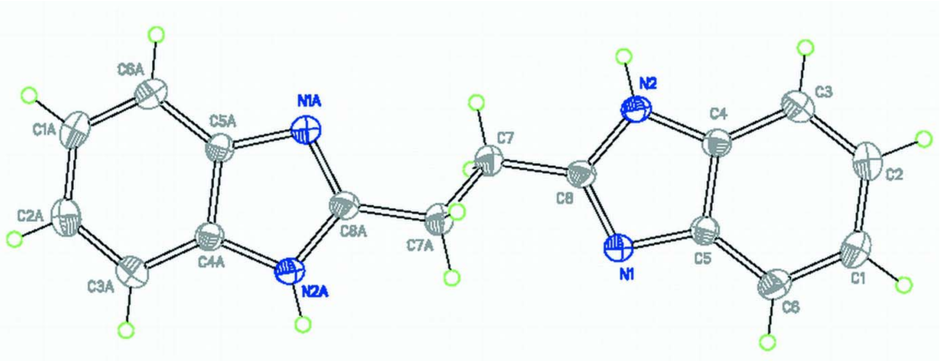

Figure 1

The molecular structure of the title compound with displacement ellipsoids drawn at the 30% probability level. Atoms with suffix A are at the symmetry position (1–x, 1–y, –z).

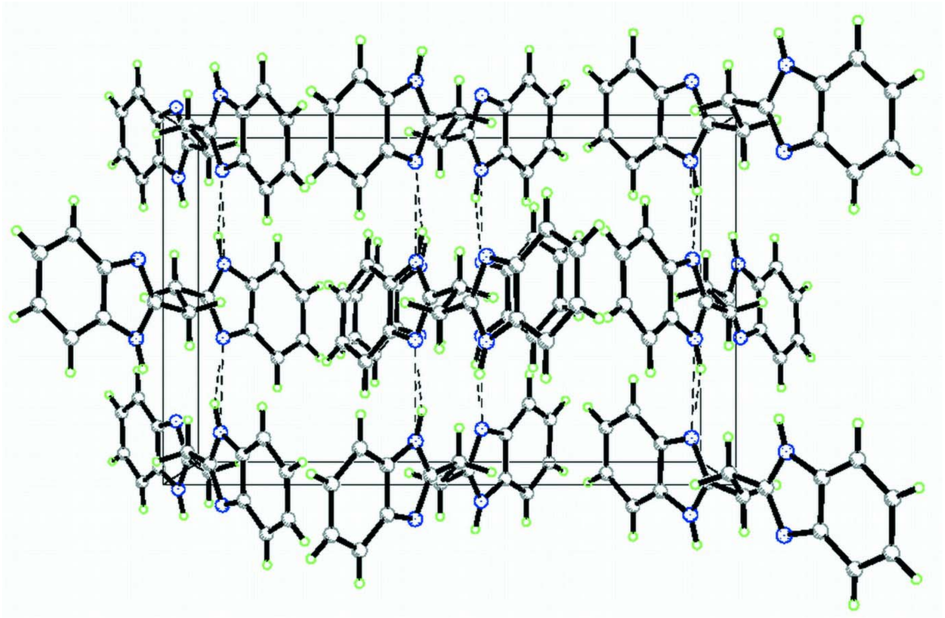

Figure 2

The stacking plot of the title compound, showing H-bond interactions (dashed lines) and π–π stacking interactions.

2,2′-(Ethane-1,2-diyl)bis(1*H*-benzimidazole)

Crystal data

$C_{16}H_{14}N_4$
$M_r = 262.31$
Orthorhombic, *Pbca*
Hall symbol: -P 2ac 2ab
$a = 8.4295\ (18)$ Å
$b = 9.924\ (2)$ Å
$c = 15.351\ (4)$ Å
$V = 1284.2\ (5)$ Å^3
$Z = 4$
$F(000) = 552$
$D_x = 1.357$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$\theta = 2.7$–$27.6°$
$\mu = 0.08$ mm^{-1}
$T = 296$ K
Block, colourless
0.32 × 0.25 × 0.19 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.975$, $T_{max} = 0.984$
10702 measured reflections
1475 independent reflections
966 reflections with $I > 2\sigma(I)$
$R_{int} = 0.052$
$\theta_{max} = 27.6°$, $\theta_{min} = 2.7°$
$h = -10 \rightarrow 10$
$k = -12 \rightarrow 12$
$l = -19 \rightarrow 16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.045$
$wR(F^2) = 0.122$
$S = 1.02$
1475 reflections
91 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	$(\Delta/\sigma)_{\max} < 0.001$
$w = 1/[\sigma^2(F_o^2) + (0.0554P)^2 + 0.2274P]$ where $P = (F_o^2 + 2F_c^2)/3$	$\Delta\rho_{\max} = 0.15$ e Å^{-3} $\Delta\rho_{\min} = -0.21$ e Å^{-3}

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	$U_{\rm iso}*/U_{\rm eq}$
N2	0.18376 (15)	0.39276 (12)	0.06131 (8)	0.0378 (4)
H2B	0.1935	0.3084	0.0498	0.045*
N1	0.23667 (16)	0.61293 (12)	0.06218 (9)	0.0402 (4)
C5	0.09915 (18)	0.58969 (15)	0.11024 (10)	0.0357 (4)
C8	0.28216 (19)	0.49246 (14)	0.03497 (11)	0.0375 (4)
C4	0.06495 (18)	0.45137 (15)	0.11012 (10)	0.0354 (4)
C7	0.42738 (19)	0.46475 (17)	−0.01726 (12)	0.0452 (4)
H7A	0.4092	0.4932	−0.0769	0.054*
H7B	0.4467	0.3684	−0.0178	0.054*
C3	−0.0631 (2)	0.39827 (18)	0.15503 (11)	0.0475 (5)
H3A	−0.0860	0.3066	0.1537	0.057*
C6	0.0040 (2)	0.67805 (16)	0.15747 (11)	0.0461 (5)
H6A	0.0247	0.7701	0.1581	0.055*
C2	−0.1552 (2)	0.48740 (18)	0.20187 (12)	0.0524 (5)
H2A	−0.2416	0.4551	0.2333	0.063*
C1	−0.1215 (2)	0.62512 (18)	0.20317 (12)	0.0520 (5)
H1A	−0.1856	0.6824	0.2357	0.062*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N2	0.0346 (8)	0.0281 (6)	0.0506 (8)	0.0003 (5)	0.0010 (6)	−0.0046 (6)
N1	0.0373 (8)	0.0317 (7)	0.0515 (8)	−0.0013 (5)	0.0053 (6)	−0.0039 (6)
C5	0.0323 (9)	0.0347 (8)	0.0402 (9)	0.0015 (7)	−0.0014 (7)	0.0005 (6)
C8	0.0328 (9)	0.0329 (8)	0.0469 (9)	−0.0014 (6)	−0.0024 (7)	−0.0044 (7)
C4	0.0326 (9)	0.0330 (8)	0.0407 (9)	0.0013 (6)	−0.0027 (7)	−0.0005 (6)
C7	0.0343 (9)	0.0450 (9)	0.0563 (11)	−0.0019 (7)	0.0050 (8)	−0.0102 (8)
C3	0.0458 (11)	0.0432 (9)	0.0537 (10)	−0.0071 (8)	0.0034 (9)	0.0023 (8)
C6	0.0473 (11)	0.0371 (9)	0.0541 (11)	0.0069 (8)	0.0020 (9)	−0.0036 (7)
C2	0.0435 (11)	0.0626 (12)	0.0512 (11)	−0.0013 (9)	0.0105 (9)	0.0027 (9)
C1	0.0458 (11)	0.0571 (11)	0.0529 (11)	0.0130 (9)	0.0083 (9)	−0.0057 (9)

Geometric parameters (Å, º)

N2—C8	1.3530 (19)	C7—H7A	0.9700
N2—C4	1.3795 (19)	C7—H7B	0.9700
N2—H2B	0.8600	C3—C2	1.379 (2)
N1—C8	1.3233 (18)	C3—H3A	0.9300
N1—C5	1.393 (2)	C6—C1	1.374 (2)
C5—C6	1.392 (2)	C6—H6A	0.9300
C5—C4	1.403 (2)	C2—C1	1.396 (2)
C8—C7	1.489 (2)	C2—H2A	0.9300
C4—C3	1.385 (2)	C1—H1A	0.9300
C7—C7$^{\text{i}}$	1.506 (3)		
C8—N2—C4	107.40 (12)	C8—C7—H7B	109.0
C8—N2—H2B	126.3	C7$^{\text{i}}$—C7—H7B	109.0
C4—N2—H2B	126.3	H7A—C7—H7B	107.8
C8—N1—C5	104.99 (12)	C2—C3—C4	117.01 (16)
C6—C5—N1	130.61 (14)	C2—C3—H3A	121.5
C6—C5—C4	119.91 (15)	C4—C3—H3A	121.5
N1—C5—C4	109.41 (13)	C1—C6—C5	117.96 (15)
N1—C8—N2	112.88 (14)	C1—C6—H6A	121.0
N1—C8—C7	125.11 (14)	C5—C6—H6A	121.0
N2—C8—C7	122.00 (13)	C3—C2—C1	121.40 (17)
N2—C4—C3	132.51 (15)	C3—C2—H2A	119.3
N2—C4—C5	105.32 (13)	C1—C2—H2A	119.3
C3—C4—C5	122.14 (15)	C6—C1—C2	121.57 (16)
C8—C7—C7$^{\text{i}}$	113.14 (16)	C6—C1—H1A	119.2
C8—C7—H7A	109.0	C2—C1—H1A	119.2
C7$^{\text{i}}$—C7—H7A	109.0		
C8—N1—C5—C6	176.72 (17)	N1—C5—C4—C3	178.13 (14)
C8—N1—C5—C4	−0.20 (18)	N1—C8—C7—C7$^{\text{i}}$	46.1 (3)
C5—N1—C8—N2	0.41 (18)	N2—C8—C7—C7$^{\text{i}}$	−132.3 (2)
C5—N1—C8—C7	−178.13 (15)	N2—C4—C3—C2	176.40 (16)
C4—N2—C8—N1	−0.47 (19)	C5—C4—C3—C2	−1.2 (2)
C4—N2—C8—C7	178.12 (14)	N1—C5—C6—C1	−176.40 (16)
C8—N2—C4—C3	−177.62 (17)	C4—C5—C6—C1	0.2 (2)
C8—N2—C4—C5	0.31 (17)	C4—C3—C2—C1	0.6 (3)
C6—C5—C4—N2	−177.37 (14)	C5—C6—C1—C2	−0.9 (3)
N1—C5—C4—N2	−0.07 (17)	C3—C2—C1—C6	0.4 (3)
C6—C5—C4—C3	0.8 (2)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*

N2—H2*B*···N1$^{\text{ii}}$	0.86	2.04	2.8568 (18)	159

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