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1,4-Bis(1*H*-benzimidazol-1-yl)but-2-ene

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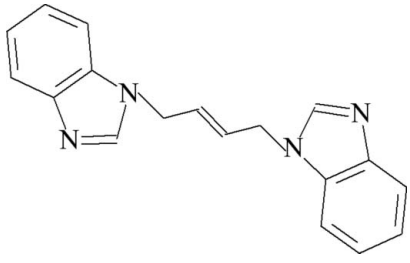
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.004 Å; R factor = 0.052; wR factor = 0.133; data-to-parameter ratio = 14.7.

In the pseudo-centrosymmetric molecule of the title compound, $C_{18}H_{16}N_4$, two benzimidazole fragments form the dihedral angles of 83.49 (7) and 79.37 (7)°, with the mean plane of the linking butene chain. No classical intermolecular interactions are observed. The porous crystal packing exhibits voids of 85 Å^3.

Related literature

For applications of benzimidazole derivatives, see: Tidwell *et al.* (1993); Santra & Dogra (1999). For related structures, see: Su *et al.* (2003); Chen *et al.* (2007); Liu *et al.* (2011).



Experimental

Crystal data

$C_{18}H_{16}N_4$
M_r = 288.35
Monoclinic, $P2_1/c$
a = 12.564 (3) Å
b = 9.140 (2) Å
c = 18.131 (3) Å
β = 127.281 (12)°
V = 1656.7 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.07 mm^{-1}
T = 295 K
0.20 × 0.18 × 0.17 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.956, T_{max} = 0.996
12226 measured reflections
2925 independent reflections
1639 reflections with $I > 2\sigma(I)$
R_{int} = 0.056

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.133
S = 1.01
2925 reflections
199 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 e Å^{-3}

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); 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: *SHELXTL* and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV5116).

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supplementary materials

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1,4-Bis(1*H*-benzimidazol-1-yl)but-2-ene

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Comment

Bis-benzimidazole compounds have have been widely used due to their anti-viral activities (Tidwell *et al.*, 1993), photochemical and photophysical properties (Santra & Dogra, 1999). They have found applications in supramolecular coordination chemistry to generate various coordination architectures (Su *et al.*, 2003; Chen *et al.*, 2007; Liu *et al.*, 2011). Herewith we report the crystal structure of the title bis-benzimidazole compound (I).

In (I) (Fig. 1), the molecule adopts a *trans* conformation. Two benzimidazole fragments form the dihedral angles of 83.49 (7) and 79.37 (7) °, respectively, with the mean plane of linking them butene chain. The C11—C10—C9—C8 torsion angle is 176.5 (3)°. The average bond distances and angles for the benzimidazole ring are in agreement with those in related benzimidazole compounds (Chen *et al.*, 2007; Liu *et al.*2011). In the absence of classical intermolecular interactions, the porous crystal packing exhibits voids of 85 Å^3.

Experimental

The title compound was prepared according to the literature (Liu *et al.*, 2011). Single crystals were grown from an ethanol solution over a period of several days at room temperature.

Refinement

H atoms were placed in calculated positions (C—H 0.93-0.97 Å), and refined with a riding model, with U_{iso}(H) = 1.2U_{eq}(C). The program Squeeze in *PLATON* (Spek, 2009) was applied to remove regions of diffuse electron density that could not be satisfactorily modeled.

Figures

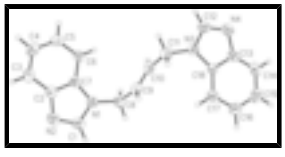


Fig. 1. The molecular structure of (I), showing displacement ellipsoids at the 30% probability level.

1,4-Bis(1*H*-benzimidazol-1-yl)but-2-ene

Crystal data

$C_{18}H_{16}N_4$	$F(000)$ = 608
M_r = 288.35	D_x = 1.156 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, λ = 0.71073 Å

Hall symbol: -P 2ybc	Cell parameters from 4528 reflections
a = 12.564 (3) Å	θ = 3.5–20.3°
b = 9.140 (2) Å	μ = 0.07 mm^{-1}
c = 18.131 (3) Å	T = 295 K
β = 127.281 (12)°	Block, colourless
V = 1656.7 (6) Å^3	0.20 × 0.18 × 0.17 mm
Z = 4	

Data collection

Bruker SMART CCD area-detector diffractometer	2925 independent reflections
Radiation source: fine–focus sealed tube	1639 reflections with $I > 2\sigma(I)$
graphite	R_{int} = 0.056
φ and ω scans	θ_{max} = 25.0°, θ_{min} = 2.0°
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	h = −14→14
T_{min} = 0.956, T_{max} = 0.996	k = −10→10
12226 measured reflections	l = −21→21

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)]$ = 0.052	Hydrogen site location: inferred from neighbouring sites
$wR(F^2)$ = 0.133	H-atom parameters constrained
S = 1.01	$w = 1/[\sigma^2(F_o^2) + (0.0545P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
2925 reflections	$(\Delta/\sigma)_{max} < 0.001$
199 parameters	$\Delta\rho_{max}$ = 0.19 e Å^{-3}
0 restraints	$\Delta\rho_{min}$ = −0.14 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_{iso}*/U_{eq}
N1	0.93808 (17)	−0.12271 (19)	0.16716 (12)	0.0514 (5)
N2	1.0262 (2)	−0.1093 (2)	0.31752 (13)	0.0646 (6)
N3	0.55655 (17)	0.1198 (2)	−0.20779 (12)	0.0533 (5)
N4	0.4402 (2)	0.1102 (2)	−0.36219 (14)	0.0724 (6)
C1	1.0390 (2)	−0.0742 (2)	0.25325 (18)	0.0632 (7)
H1	1.1111	−0.0206	0.2655	0.076*
C2	0.9075 (2)	−0.1874 (2)	0.27030 (15)	0.0528 (6)
C3	0.8415 (3)	−0.2500 (3)	0.30264 (17)	0.0650 (7)
H3	0.8766	−0.2436	0.3648	0.078*
C4	0.7230 (3)	−0.3217 (3)	0.2396 (2)	0.0710 (7)
H4	0.6771	−0.3641	0.2595	0.085*
C5	0.6706 (2)	−0.3319 (3)	0.14720 (18)	0.0662 (7)
H5	0.5907	−0.3822	0.1068	0.079*
C6	0.7322 (2)	−0.2708 (2)	0.11317 (16)	0.0567 (6)
H6	0.6962	−0.2778	0.0509	0.068*
C7	0.8516 (2)	−0.1974 (2)	0.17686 (14)	0.0474 (6)
C8	0.9207 (2)	−0.0957 (2)	0.08116 (15)	0.0592 (6)
H8A	0.8973	−0.1865	0.0469	0.071*
H8B	1.0043	−0.0612	0.0955	0.071*
C9	0.8136 (2)	0.0152 (3)	0.02248 (17)	0.0590 (6)
H9	0.8277	0.1096	0.0460	0.071*
C10	0.7016 (2)	−0.0108 (2)	−0.05950 (17)	0.0600 (6)
H10	0.6902	−0.1037	−0.0843	0.072*
C11	0.5908 (2)	0.0964 (3)	−0.11649 (16)	0.0678 (7)
H11B	0.5122	0.0616	−0.1235	0.081*
H11A	0.6166	0.1892	−0.0839	0.081*
C12	0.4456 (2)	0.0739 (3)	−0.2902 (2)	0.0684 (7)
H12	0.3783	0.0207	−0.2953	0.082*
C13	0.5584 (2)	0.1877 (2)	−0.32404 (15)	0.0548 (6)
C14	0.6068 (3)	0.2551 (3)	−0.36690 (17)	0.0738 (8)
H14	0.5599	0.2508	−0.4308	0.089*
C15	0.7263 (3)	0.3282 (3)	−0.3115 (2)	0.0797 (8)
H15	0.7597	0.3761	−0.3388	0.096*
C16	0.7985 (2)	0.3327 (3)	−0.2160 (2)	0.0699 (7)
H16	0.8794	0.3827	−0.1807	0.084*
C17	0.7535 (2)	0.2653 (2)	−0.17234 (16)	0.0545 (6)
H17	0.8021	0.2673	−0.1082	0.065*
C18	0.6318 (2)	0.1941 (2)	−0.22858 (14)	0.0443 (5)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0494 (11)	0.0484 (11)	0.0549 (12)	−0.0002 (9)	0.0308 (11)	0.0018 (9)
N2	0.0630 (13)	0.0578 (13)	0.0591 (13)	−0.0018 (11)	0.0297 (11)	−0.0044 (10)

N3	0.0467 (11)	0.0536 (12)	0.0573 (12)	0.0023 (10)	0.0303 (10)	0.0052 (10)
N4	0.0592 (14)	0.0724 (15)	0.0568 (13)	−0.0074 (12)	0.0201 (11)	−0.0030 (11)
C1	0.0531 (15)	0.0533 (16)	0.0684 (18)	−0.0049 (12)	0.0291 (15)	−0.0048 (13)
C2	0.0570 (15)	0.0439 (13)	0.0556 (15)	0.0049 (12)	0.0331 (13)	−0.0007 (11)
C3	0.084 (2)	0.0591 (16)	0.0631 (16)	0.0103 (14)	0.0507 (16)	0.0061 (12)
C4	0.0794 (19)	0.0583 (17)	0.094 (2)	0.0030 (15)	0.0625 (18)	0.0055 (15)
C5	0.0515 (15)	0.0570 (16)	0.084 (2)	−0.0026 (13)	0.0376 (15)	0.0007 (13)
C6	0.0537 (15)	0.0529 (15)	0.0532 (14)	0.0025 (12)	0.0269 (13)	0.0030 (11)
C7	0.0455 (13)	0.0417 (13)	0.0488 (14)	0.0046 (11)	0.0253 (12)	0.0022 (10)
C8	0.0641 (15)	0.0595 (15)	0.0607 (15)	0.0039 (13)	0.0413 (13)	0.0064 (12)
C9	0.0732 (16)	0.0531 (15)	0.0619 (16)	0.0067 (13)	0.0468 (15)	0.0067 (12)
C10	0.0753 (17)	0.0540 (15)	0.0641 (16)	0.0089 (14)	0.0492 (15)	0.0122 (12)
C11	0.0686 (17)	0.0706 (17)	0.0766 (18)	0.0148 (14)	0.0504 (15)	0.0169 (13)
C12	0.0478 (15)	0.0543 (16)	0.082 (2)	−0.0080 (12)	0.0285 (16)	0.0017 (14)
C13	0.0522 (15)	0.0512 (14)	0.0527 (14)	0.0033 (12)	0.0274 (13)	−0.0001 (11)
C14	0.083 (2)	0.082 (2)	0.0539 (16)	0.0163 (16)	0.0402 (16)	0.0155 (14)
C15	0.080 (2)	0.079 (2)	0.105 (2)	0.0119 (17)	0.0691 (19)	0.0235 (17)
C16	0.0555 (15)	0.0593 (17)	0.092 (2)	−0.0005 (13)	0.0430 (16)	0.0075 (14)
C17	0.0485 (14)	0.0457 (14)	0.0588 (15)	0.0036 (11)	0.0271 (13)	0.0026 (11)
C18	0.0420 (13)	0.0384 (12)	0.0490 (14)	0.0039 (11)	0.0258 (11)	0.0027 (10)

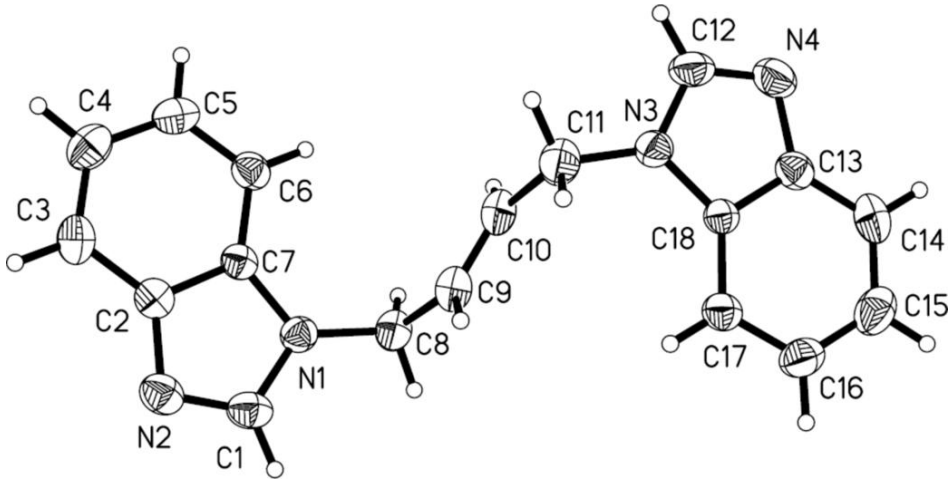
Geometric parameters (Å, °)

N1—C1	1.358 (3)	C8—C9	1.495 (3)
N1—C7	1.382 (2)	C8—H8A	0.9700
N1—C8	1.458 (2)	C8—H8B	0.9700
N2—C1	1.309 (3)	C9—C10	1.308 (3)
N2—C2	1.387 (3)	C9—H9	0.9300
N3—C12	1.352 (3)	C10—C11	1.491 (3)
N3—C18	1.389 (2)	C10—H10	0.9300
N3—C11	1.452 (3)	C11—H11B	0.9700
N4—C12	1.308 (3)	C11—H11A	0.9700
N4—C13	1.393 (3)	C12—H12	0.9300
C1—H1	0.9300	C13—C18	1.384 (3)
C2—C7	1.389 (3)	C13—C14	1.387 (3)
C2—C3	1.395 (3)	C14—C15	1.372 (3)
C3—C4	1.375 (3)	C14—H14	0.9300
C3—H3	0.9300	C15—C16	1.387 (3)
C4—C5	1.383 (3)	C15—H15	0.9300
C4—H4	0.9300	C16—C17	1.365 (3)
C5—C6	1.368 (3)	C16—H16	0.9300
C5—H5	0.9300	C17—C18	1.383 (3)
C6—C7	1.391 (3)	C17—H17	0.9300
C6—H6	0.9300		
C1—N1—C7	105.92 (18)	H8A—C8—H8B	108.0
C1—N1—C8	127.2 (2)	C10—C9—C8	124.8 (2)
C7—N1—C8	126.83 (18)	C10—C9—H9	117.6
C1—N2—C2	104.1 (2)	C8—C9—H9	117.6
C12—N3—C18	105.52 (19)	C9—C10—C11	125.3 (2)

C12—N3—C11	127.5 (2)	C9—C10—H10	117.3
C18—N3—C11	126.95 (19)	C11—C10—H10	117.3
C12—N4—C13	103.8 (2)	N3—C11—C10	113.18 (19)
N2—C1—N1	114.2 (2)	N3—C11—H11B	108.9
N2—C1—H1	122.9	C10—C11—H11B	108.9
N1—C1—H1	122.9	N3—C11—H11A	108.9
N2—C2—C7	110.3 (2)	C10—C11—H11A	108.9
N2—C2—C3	130.0 (2)	H11B—C11—H11A	107.8
C7—C2—C3	119.7 (2)	N4—C12—N3	114.8 (2)
C4—C3—C2	117.8 (2)	N4—C12—H12	122.6
C4—C3—H3	121.1	N3—C12—H12	122.6
C2—C3—H3	121.1	C18—C13—C14	119.7 (2)
C3—C4—C5	121.3 (2)	C18—C13—N4	110.2 (2)
C3—C4—H4	119.3	C14—C13—N4	130.1 (2)
C5—C4—H4	119.3	C15—C14—C13	117.6 (2)
C6—C5—C4	122.3 (2)	C15—C14—H14	121.2
C6—C5—H5	118.8	C13—C14—H14	121.2
C4—C5—H5	118.8	C14—C15—C16	121.7 (2)
C5—C6—C7	116.3 (2)	C14—C15—H15	119.1
C5—C6—H6	121.9	C16—C15—H15	119.1
C7—C6—H6	121.9	C17—C16—C15	121.6 (2)
N1—C7—C2	105.48 (19)	C17—C16—H16	119.2
N1—C7—C6	131.9 (2)	C15—C16—H16	119.2
C2—C7—C6	122.6 (2)	C16—C17—C18	116.5 (2)
N1—C8—C9	111.31 (18)	C16—C17—H17	121.8
N1—C8—H8A	109.4	C18—C17—H17	121.8
C9—C8—H8A	109.4	C17—C18—C13	122.9 (2)
N1—C8—H8B	109.4	C17—C18—N3	131.3 (2)
C9—C8—H8B	109.4	C13—C18—N3	105.72 (19)
C2—N2—C1—N1	0.1 (3)	C12—N3—C11—C10	108.2 (3)
C7—N1—C1—N2	−0.3 (2)	C18—N3—C11—C10	−71.6 (3)
C8—N1—C1—N2	176.94 (19)	C9—C10—C11—N3	123.4 (2)
C1—N2—C2—C7	0.2 (2)	C13—N4—C12—N3	−0.2 (3)
C1—N2—C2—C3	−178.6 (2)	C18—N3—C12—N4	−0.1 (3)
N2—C2—C3—C4	179.6 (2)	C11—N3—C12—N4	−179.9 (2)
C7—C2—C3—C4	0.8 (3)	C12—N4—C13—C18	0.4 (2)
C2—C3—C4—C5	0.2 (3)	C12—N4—C13—C14	−178.9 (2)
C3—C4—C5—C6	−0.7 (4)	C18—C13—C14—C15	−1.1 (3)
C4—C5—C6—C7	0.2 (3)	N4—C13—C14—C15	178.1 (2)
C1—N1—C7—C2	0.4 (2)	C13—C14—C15—C16	1.4 (4)
C8—N1—C7—C2	−176.86 (18)	C14—C15—C16—C17	−0.5 (4)
C1—N1—C7—C6	−179.6 (2)	C15—C16—C17—C18	−0.7 (3)
C8—N1—C7—C6	3.1 (3)	C16—C17—C18—C13	1.0 (3)
N2—C2—C7—N1	−0.4 (2)	C16—C17—C18—N3	−177.8 (2)
C3—C2—C7—N1	178.58 (19)	C14—C13—C18—C17	−0.1 (3)
N2—C2—C7—C6	179.66 (19)	N4—C13—C18—C17	−179.48 (19)
C3—C2—C7—C6	−1.3 (3)	C14—C13—C18—N3	178.9 (2)
C5—C6—C7—N1	−179.1 (2)	N4—C13—C18—N3	−0.4 (2)
C5—C6—C7—C2	0.8 (3)	C12—N3—C18—C17	179.2 (2)

C1—N1—C8—C9	−104.7 (2)	C11—N3—C18—C17	−0.9 (3)
C7—N1—C8—C9	72.0 (3)	C12—N3—C18—C13	0.3 (2)
N1—C8—C9—C10	−116.2 (2)	C11—N3—C18—C13	−179.85 (19)
C8—C9—C10—C11	176.37 (19)		

Fig. 1


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