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1,4-Bis(2-benzimidazolyl)benzene

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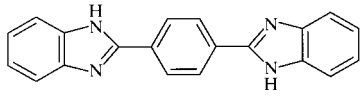
The title compound, $C_{20}H_{14}N_4$, lies about an inversion centre and the benzimidazole moiety and the phenyl ring are twisted by 30.9 (1)°. The benzimidazole moiety is completely planar, with a maximum deviation of 0.009 (2) Å. Intermolecular N—H···N hydrogen bonds give rise to a layered structure, with the layers stacked by van der Waals interactions.

Comment

Benzimidazole is an interesting heterocyclic ring because it is present in various naturally occurring drugs such as omeprazole, astemizole and emedastine difumarate (Sakai *et al.*, 1989). The efficacy of substituted benzimidazoles in the treatment of parasitic infections is well known (Brown *et al.*, 1961; Preston, 1974; Sarkar *et al.*, 1984). Substituted benzimidazole moieties are established pharmacophores in parasitic chemotherapy. Bis(2-benzimidazoles) and some substituted bis(2-benzimidazolyl)alkanes have attracted much interest because of their wide-ranging antiviral activity (Tidwell *et al.*, 1993) and also because of the coordination chemistry of azoles acting as ligands in transition metal compounds. Such compounds are increasingly being studied in the context of modelling biological systems (Bouwman *et al.*, 1990; Pujar & Bharamgoudar, 1988). The present work reports the crystal and molecular structure of the title compound, (I).



(I)

The asymmetric unit contains half the molecule and the other half is inversion related (Fig. 1) ($1-x, -y, 1-z$). The average bond distances and angles for the benzimidazole ring is in good agreement with those of other substituted bis(benzimidazole) compounds (Matthews *et al.*, 1996; Ozbey *et al.*, 1998). The two internal-ring bond angles, at C7 [113.3 (2)°] and at C8 [119.2 (2)°], are similar to those found in related compounds (Rajnikant *et al.*, 1995). The C7—C8 bond length, 1.468 (3) Å, is close to the standard value for a single-bond length between trigonally linked C atoms (Cruickshank & Sparks, 1960). The bond lengths of C—N in the imidazole ring are in the range 1.320–1.400 Å, which are shorter than the single-bond length of 1.48 Å and longer than the typical C═N distance of 1.28 Å, indicating partial double-bond character. This can be interpreted in terms of conjugation in the heterocycle. The phenyl ring is twisted through 30.9 (1)° with the benzimidazole moiety along the C7—C8 bond. The benzimidazole moiety is completely planar, with a maximum deviation of 0.009 (2)° for C2; the dihedral angle between the aromatic ring and the five-membered ring is only 0.1 (1)°.

The molecule forms a two-dimensional network bonded through intermolecular N—H···N hydrogen bonds. The hydrogen-bonded layers, parallel to (001), are stacked upon one another by translation and held together by van der Waals attractions.

Experimental

The title compound was prepared from benzene-1,4-dicarboxylic acid and 1,2-diaminobenzene in 66% yield using a modified Phillips reaction (Addison & Burke, 1981; Addison *et al.*, 1983) and was recrystallized from methanol. The single crystals suitable for X-ray analysis were then obtained by slow evaporation at room temperature from the EtOH solvent.

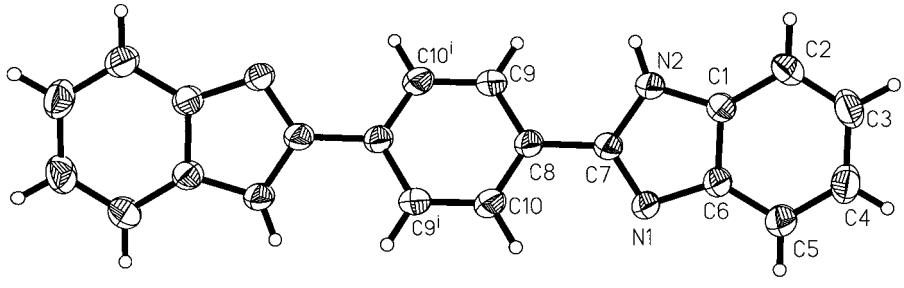


Figure 1
The structure of (I) showing 50% probability displacement ellipsoids and the atom-numbering scheme [symmetry code: (i) $1-x, -y, 1-z$].

Crystal data

$C_{20}H_{14}N_4$
M_r = 310.35
Orthorhombic, *Pbca*
a = 10.2400 (3) Å
b = 9.7505 (2) Å
c = 15.0310 (4) Å
V = 1500.77 (7) Å^3
Z = 4
D_x = 1.374 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3853 reflections
θ = 2.71–28.32°
μ = 0.085 mm^{-1}
T = 293 (2) K
Needle, dark red
0.50 × 0.12 × 0.10 mm

Data collection

Siemens SMART CCD area-detector diffractometer
ω scans
9577 measured reflections
1846 independent reflections
1223 reflections with $I > 2\sigma(I)$
R_{int} = 0.076
θ_{max} = 28.28°
$h = -9 \rightarrow 13$
$k = -12 \rightarrow 12$
$l = -19 \rightarrow 19$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.067
$wR(F^2)$ = 0.155
S = 1.117
1846 reflections
109 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0584P)^2 + 0.4289P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.185 e Å^{-3}
$\Delta\rho_{min}$ = −0.298 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

N1—C7	1.320 (3)	C8—C10	1.386 (3)
N1—C6	1.400 (3)	C8—C9	1.398 (3)
N2—C7	1.359 (2)	C9—C10^{i}	1.377 (3)
N2—C1	1.379 (3)	C10—C9^{i}	1.377 (3)
C7—N1—C6	104.4 (2)	C7—N2—C1	107.0 (2)

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 1990).

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···N1^{i}	0.86	2.17	3.033 (2)	175

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

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: SK1369). A packing diagram of (I) has also been deposited. Services for accessing these data are described at the back of the journal.

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