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1,1′-Butane-1,4-diylbis(1*H*-benzimidazole)

Mehmet Akkurt,[a]* Selvi Karaca,[a] Hasan Küçükbay[b] and Orhan Büyükgüngör[c]

[a]Department of Physics, Faculty of Arts and Sciences, Erciyes University, 38039 Kayseri, Turkey, [b]Department of Chemistry, Faculty of Arts and Sciences, İnönü University, 44280 Malatya, Turkey, and [c]Department of Physics, Faculty of Arts and Sciences, Ondokuz Mayıs University, 55139 Samsun, Turkey

Correspondence e-mail: akkurt@erciyes.edu.tr

Key indicators

Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.002 Å
R factor = 0.031
wR factor = 0.085
Data-to-parameter ratio = 17.8

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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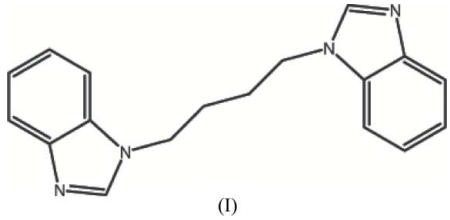
The molecule of the title compound, $C_{18}H_{18}N_4$, is disposed about a center of inversion. The dihedral angle between the five- and six-membered rings is 1.23 (6)°, showing almost exact coplanarity.

Comment

Benzimidazole and its derivatives have been reported to have a broad scope of biological activity. For example, they have been found to be essential in the biosynthesis of purine nucleotides and long-chain fatty acids (Khalil *et al.*, 2001). Bis-benzimidazole compounds have received much attention for their wide-ranging anti-viral activities (Tidwell *et al.*, 1993), antimicrobial properties (Küçükbay *et al.*, 1995, 2001), photochemical and photophysical properties (Santra & Dogra, 1999), their importance in selective ion-exchange resins (Albada *et al.*, 2002) and their ability to form supramolecular aggregates with transition metal ions (Su *et al.*, 2001). In the light of the general importance of benzimidazole compounds, the study of bis-benzimidazole derivatives is still an important area of research. The objective of this study was to elucidate the structure of the title bis-benzimidazole, (I), which was synthesized by a different method from that described in the literature (Gök, 1999).



(I)

Molecule (I) (Fig. 1) lies about an inversion center at the mid-point of C9—C9^{i} [symmetry code: (i) $1-x, -y, 1-z$]. The N1—C8, C8—C9, and C9—C9^{i} bond lengths (Table 1) are all close to the standard value for a single-bond length (Allen *et al.*, 1987). The average bond distances and angles for the benzimidazole ring are in agreement with those of our previous studies on related benzimidazole compounds (Öztürk *et al.*, 2003; Akkurt, Pınar *et al.*, 2006; Akkurt, Yıldırım *et al.*, 2006) and the literature (Chen *et al.*, 2002; Allen *et al.*, 1987). The benzimidazole ring system is almost planar, with maximum deviations of −0.014 (1) and 0.018 (1) Å, respectively for atoms N1 and N2.

Experimental

To a solution of benzimidazole (3 g, 25.42 mmol) in THF (30 ml) was added metallic Na (6.4 g, 27.97 mmol) and the mixture was stirred for

10 h at room temperature. 1,4-Dibromobutane (1.6 ml, 13.34 mmol) was added to the reaction mixture which was then stirred for 5 h at room temperature. All volatiles were removed *in vacuo* and water was added to precipitate the product. The crude product was crystallized from a toluene/*n*-hexane (3:1) mixture which, upon cooling to 253 K, gave crystals (yield: 3.06 g, 83%; m.p. 448–449 K). ^{1}H NMR ($CDCl_3$): δ 2.37 (*m*, $-CH_2-CH_2-$, 2H), 4.69 (*t*, $-CH_2-N$, 2H), 7.83–7.98 (*m*, Ar–H, 4H), 8.63 (*s*, N–CH–N, 1H). Analysis calculated for $C_{18}H_{18}N_4$: C 74.48, H 6.21, N 19.31%; found: C 74.52, H 6.21, N 19.43%.

Crystal data

$C_{18}H_{18}N_4$
M_r = 290.36
Monoclinic, $P2_1/c$
a = 5.6495 (4) Å
b = 10.6323 (7) Å
c = 12.7814 (9) Å
β = 99.042 (6)°
V = 758.20 (9) Å^3
Z = 2
D_x = 1.272 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 296 K
Prism, colorless
0.43 × 0.35 × 0.27 mm

Data collection

Stoe IPDS-2 diffractometer
ω scans
Absorption correction: none
11438 measured reflections
1795 independent reflections
1354 reflections with $I > 2\sigma(I)$
R_{int} = 0.062
θ_{max} = 27.9°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.085
S = 1.04
1795 reflections
101 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0449P)^2 + 0.023P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.13 e Å^{-3}
$\Delta\rho_{min}$ = −0.11 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.086 (8)

Table 1
Selected geometric parameters (Å, °).

N1—C1	1.3564 (13)	N2—C1	1.3079 (14)
N1—C7	1.3772 (13)	N2—C2	1.3853 (13)
N1—C8	1.4597 (13)		
C1—N1—C7	106.30 (8)	N2—C2—C3	130.29 (9)
C1—N1—C8	127.13 (9)	N2—C2—C7	110.27 (9)
C7—N1—C8	126.24 (8)	N1—C7—C2	105.04 (8)
C1—N2—C2	103.98 (8)	N1—C7—C6	132.15 (9)
N1—C1—N2	114.40 (9)	N1—C8—C9	111.88 (9)

H atoms were included in the riding-model approximation, with C—H = 0.93–0.97 Å and U_{iso}(H) = 1.2U_{eq}(C).

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

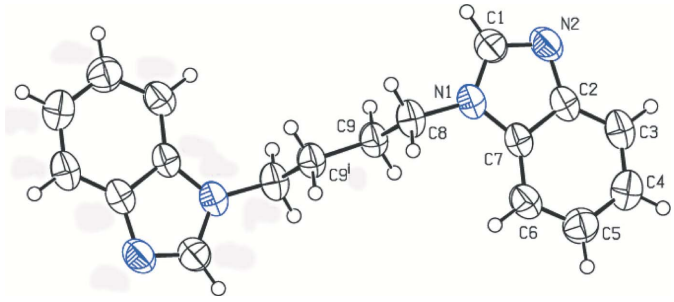


Figure 1
The molecular structure of (I), showing the atom-labeling scheme and displacement ellipsoids drawn at the 50% probability level. [Symmetry code: (i) $1-x, -y, 1-z$.]

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