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3,3′-(4-Bromophenylmethanediyl)bis(5-methoxy-1*H*-indole)

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.007 Å
R factor = 0.058
wR factor = 0.135
Data-to-parameter ratio = 15.4

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

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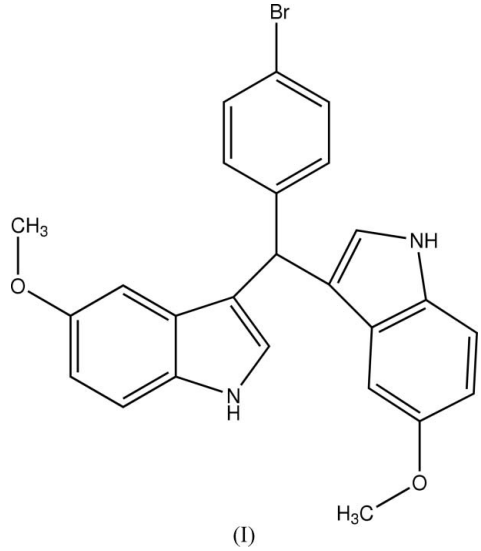
The title compound, $C_{25}H_{21}BrN_2O_2$, was synthesized by the reaction of 5-methoxy-1*H*-indole and 4-bromobenzaldehyde in ethanol, using $CuBr_2$ as a catalyst under microwave irradiation. In the crystal structure, there is an intermolecular N—H···O hydrogen bond and two intermolecular C—H···π contacts.

Comment

Development of bis(indolyl)alkane synthesis has been of considerable interest because of the wide occurrence of bis-(indolyl)alkanes in various natural products possessing biological activity (Bell *et al.*, 1994) and their usefulness for drug design. We report here the crystal structure of the title compound, (I).



(I)

The molecular structure of compound (I) is shown in Fig. 1. Bond lengths and angles are within normal ranges (Allen *et al.*, 1987). Ring *A* comprises atoms C20–C25, ring *B* atoms C5/N1/C6/C7/C8 and ring *C* atoms C14/N2/C15/C16/C17. The various dihedral angles are *A*/*C* = 92.8 (2), *B*/*C* = 100.8 (1) and *A*/*B* = 81.6 (2)°.

The crystal structure of (I) is stabilized by one intermolecular N—H···O contact and two intermolecular C—H···π contacts (Table 1). The N—H···O hydrogen bond and C—H···π contacts are also present in the chloro analogue (Zhang *et al.*, 2006).

Experimental

Compound (I) was prepared by the reaction of 5-methoxy-1*H*-indole (20 mmol) with 4-bromobenzaldehyde (10 mmol) in ethanol (5 ml),

using $CuBr_2$ (0.446 g) as catalyst under microwave irradiation (280 W) for 10 min. After completion, the reaction mixture was quenched with H_2O (10 ml) and extracted with EtOAc (3 × 10 ml). The combined organic layers were dried over Na_2SO_4, concentrated, and purified by column chromatography on SiO_2 (ethyl acetate–petroleum ether, 1:3 *v*/*v*) to afford the pure product (I). Crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation of a methanol solution.

Crystal data

$C_{25}H_{21}BrN_2O_2$
M_r = 461.35
Monoclinic, $P2_1/n$
a = 11.227 (2) Å
b = 10.382 (2) Å
c = 18.246 (4) Å
β = 90.06 (3)°
V = 2126.7 (7) Å^3
Z = 4
D_x = 1.441 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 1.96 mm^{-1}
T = 293 (2) K
Block, green
0.30 × 0.20 × 0.20 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.591, T_{max} = 0.696
4170 measured reflections
4170 independent reflections
1986 reflections with $I > 2\sigma(I)$
θ_{max} = 26.0°
3 standard reflections
every 200 reflections
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.135
S = 0.94
4170 reflections
271 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0583P)^2 + 0.0001P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···O1^{i}	0.86	2.35	2.973 (5)	129
C1—H1D···$Cg1^{ii}$	0.96	2.78	3.646 (3)	126
C24—H24A···$Cg2^{iii}$	0.93	2.74	3.608 (4)	157

Symmetry codes: (i) $x+1, y, z$; (ii) $-x+\frac{3}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$; (iii) $-x+\frac{1}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$. $Cg1$ and $Cg2$ denote the centroids of the C2–C5/C8/C9 and C14/N2/C15–C17 rings, respectively

All H atoms were placed in idealized positions and refined as riding, with C—H = 0.93–0.98 Å and N—H = 0.86 Å, and with U_{iso}(H) = xU_{eq}(parent atom), where x = 1.5 for methyl and 1.2 for all other H atoms.

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Siemens, 1996); software used to prepare material for publication: *SHELXTL*.

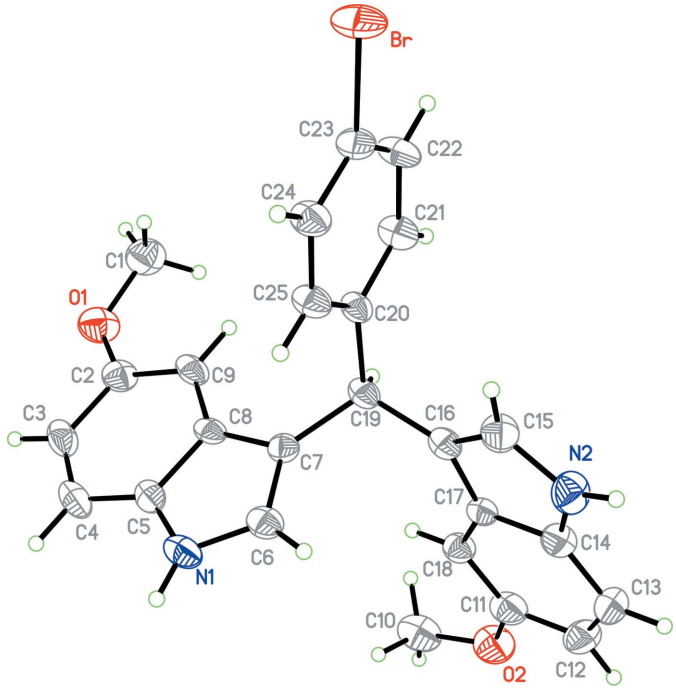


Figure 1
The molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

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