Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# 2-(2-Methoxynaphthalen-1-yl)-1-[(2-methoxynaphthalen-1-yl)methyl]-1*H*-benzimidazole

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**Key indicators**

Single-crystal X-ray study
*T* = 297 K
Mean σ(C–C) = 0.002 Å
*R* factor = 0.041
*wR* factor = 0.114
Data-to-parameter ratio = 14.9

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

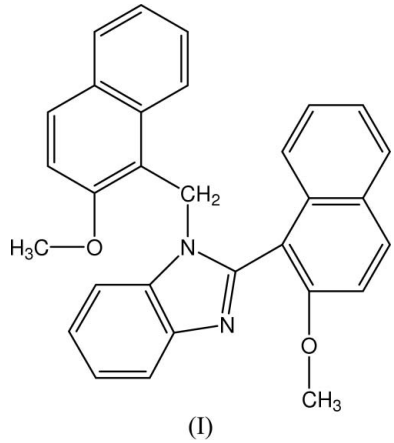


Received 9 November 2006
Accepted 18 December 2006

The folded molecular conformation of the title compound, $C_{30}H_{24}N_2O_2$, is described by the dihedral angles between the benzimidazole ring system and the naphthalene ring systems of 68.2 (1) and 78.4 (1)°. The crystal structure reveals π–π and C—H···π interactions.

## Comment

The synthesis of benzimidazoles has received much attention owing to their various biological activities such as antidiabetic (Minoura *et al.*, 2004), antimicrobial, antifungal (Pawar *et al.*, 2004), antiviral (Tomei *et al.*, 2003), anti-HIV (Rao *et al.*, 2003), and anticancer (Demirayak *et al.*, 2002). Considering the biological importance of benzimidazole derivatives, we present here the crystal structure of (I) (Fig. 1).




(I)

The bond lengths and angles in (I) are in agreement with standard values (Allen *et al.*, 1987). The overall molecular conformation can be also described by dihedral angles between the C12–C17/N2/C11/N1 and C1–C10 ring systems of 68.2 (1)°, and between the C12–C17/N2/C11/N1 and C19–C28 ring systems of 78.4 (1)°. The two methoxy groups are almost coplanar with the attached rings, as shown by the C29—O1—C1—C2 and C30—O2—C28—C27 torsion angles of 2.5 (2) and −6.6 (3)°, respectively.

An intramolecular C—H···O hydrogen bond (Table 2, Fig. 1) generates an *S*(5) ring motif (Bernstein *et al.*, 1995). The crystal structure reveals π–π and C—H···π interactions (Tables 1 and 2, Fig. 2).

## Experimental

To a solution of *o*-phenylenediamine (0.216 g, 2 mmol) in ethanol (30 ml) was added 2-methoxy-1-naphthaldehyde (0.744 g, 4 mmol).

The mixture was refluxed with stirring for 30 min in the presence of $MnCl_2{\cdot}4H_2O$ (0.197 g, 1 mmol). The resultant yellow solution was filtered. Yellow crystals suitable for X-ray structure analysis were formed after several weeks of slow evaporation of the solvent at room temperature (m.p. 445–447 K). IR spectra (KBr, $cm^{-1}$): $\nu$(C—H) 2975, 2937, $\nu$(C═N) 1619, $\nu$(C═C) 1592, 1512, $\nu$(C—N) 1251.

*Crystal data*

$C_{30}H_{24}N_2O_2$
$M_r$ = 444.51
Monoclinic, $P2_1/c$
$a$ = 8.9610 (4) Å
$b$ = 21.2905 (10) Å
$c$ = 13.5969 (5) Å
$\beta$ = 118.222 (2)°
$V$ = 2285.69 (17) Å$^3$
$Z$ = 4
$D_x$ = 1.292 Mg m$^{-3}$
Mo $K\alpha$ radiation
$\mu$ = 0.08 mm$^{-1}$
$T$ = 297 (2) K
Block, yellow
0.60 × 0.58 × 0.43 mm

*Data collection*

Bruker SMART APEX2 CCD diffractometer
$\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min}$ = 0.953, $T_{max}$ = 0.966
17482 measured reflections
4615 independent reflections
3628 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.026
$\theta_{max}$ = 26.5°

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.114
$S$ = 1.05
4615 reflections
309 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0525P)^2 + 0.4029P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.22 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.19 e Å$^{-3}$

**Table 1**
$\pi$–$\pi$ interactions (Å).

*Cg*1, *Cg*2, *Cg*3 and *Cg*4 are the centroids of the C1–C4/C9–C10, C4–C9, C19–C20/C25–C28 and C20–C25 rings, respectively.

| | | | |
|---|---|---|---|
| *Cg*1—*Cg*1$^{i}$ | 3.696 (1) | *Cg*3—*Cg*4$^{ii}$ | 3.751 (1) |
| *Cg*1—*Cg*2$^{i}$ | 3.625 (1) | | |

Symmetry codes: (i) $-x, -y+1, -z+2$; (ii) $-x, -y+1, -z+1$.

**Table 2**
Hydrogen-bond geometry (Å, °).

*Cg*1, *Cg*4 and *Cg*5 are the centroids of the C1–C4/C9–C10, C20–C25 and N1/C11/N2/C17/C12 rings, respectively.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C18—H18*B*···O2 | 0.97 | 2.27 | 2.748 (2) | 110 |
| C2—H2*A*···*Cg*4$^{iii}$ | 0.93 | 3.10 | 3.879 (2) | 143 |
| C26—H26*A*···*Cg*1$^{ii}$ | 0.93 | 3.08 | 3.744 (2) | 130 |
| C30—H30*A*···*Cg*5$^{iv}$ | 0.96 | 2.85 | 3.757 (3) | 159 |

Symmetry codes: (ii) $-x, -y+1, -z+1$; (iii) $x-1, y, z$; (iv) $x, -y+\frac{1}{2}, z-\frac{1}{2}$.

H atoms were positioned geometrically and treated as riding, with C—H = 0.93 − 0.97 Å and $U_{iso}$(H) = 1.2$U_{eq}$(C) or 1.5$U_{eq}$(methyl C).

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2005); program(s) used to solve structure: *SHELXTL* (Sheldrick, 1998); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2003).

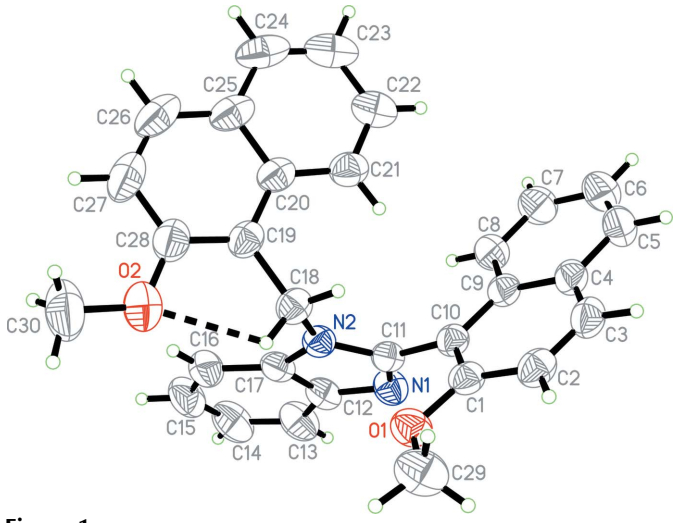



**Figure 1**
The molecular structure of (I) showing 50% probability displacement ellipsoids and the atomic numbering. The intramolecular hydrogen bond is shown as a dashed line.

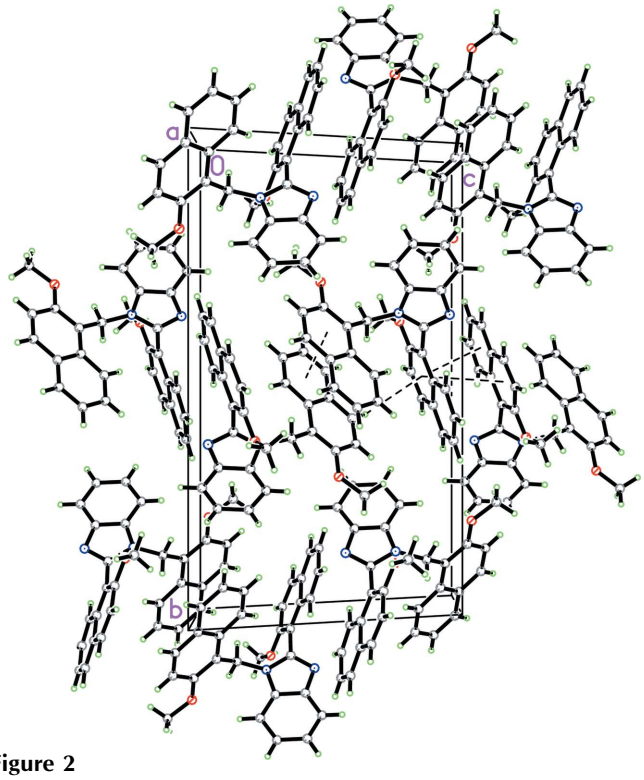



**Figure 2**
The crystal packing of (I), viewed down the *a* axis. Dashed lines indicate C—H···$\pi$ and $\pi$···$\pi$ interactions.

The authors thank the Malaysian Government, Academy of Sciences Malaysia and Universiti Sains Malaysia for the research grant and facilities. The International University of Africa (Sudan) is acknowledged for providing study leave to NEE.

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