organic papers

3,3-Bis(1H-indol-3-yl)indolin-2-one

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In the title compound, $C_{24}H_{17}N_3O$, the dihedral angles between the planes of the two indole ring systems and the oxindole group are 77.7 (1) and 71.9 (1)°. The molecular packing in the crystal structure is stabilized by an intermolecular N—H···O hydrogen bond.

Comment

Indole, being an integral part of many natural products of therapeutic importance, possesses potentially reactive sites for a variety of chemical reactions to generate molecular diversity (Farhanullah *et al.*, 2004). Indole derivatives are identified as interfering with a G protein-independent signaling pathway of the CRTH2 receptor (Mathiesen *et al.*, 2005). These derivatives also possess antiviral (Sechi *et al.*, 2004) and antimalarial (Agarwal *et al.*, 2005) activities. Oxindole derivatives possess antifungal activity (Strigacova *et al.*, 2001) and act as orally active potent growth hormone secretagogues (Tokunaga *et al.*, 2001). In view of its importance and to obtain more detailed information about the structural conformation of the molecule, the structure of the title compound, (I), was determined.

(I)
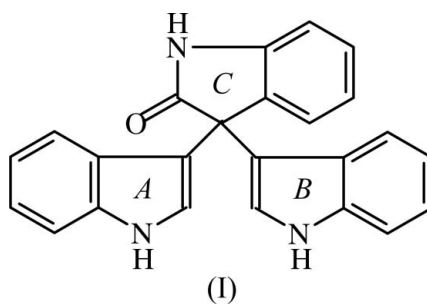
Compound (I) (Fig. 1) consists of two indole groups (*A* and *B*) and one oxindole group (*C*). Selected geometric parameters are presented in Table 1. The geometry of the indole rings is comparable to those reported for other indole derivatives (Karthick *et al.*, 2005; Sonar *et al.*, 2005).

The two indole ring systems are oriented with a dihedral angle of 68.4 (1)° with respect to each other. The dihedral angles between the oxindole plane and the indole planes (*A* and *B*) are 77.7 (1) and 71.9 (1)°, respectively.

In the crystal structure, two inversion-related molecules are linked *via* an N1—H1···O1[i] hydrogen bond (Table 2); as a result, an $R_2^2(14)$ graph-set dimer is formed.

Experimental

A mixture of indole (2.5 mmol), isatin (1.25 mmol) and gadolinium trifluoromethanesulfonate (55 mg, 0.093 mmol) was stirred in acet-

onitrile (6 ml). After completion of the reaction, water was added to quench the reaction, and the product was extracted with ethyl acetate (3 × 10 ml) and washed with aqueous sodium bicarbonate and a sodium chloride solution; the combined organic layers were dried using anhydrous Na_2SO_4 and filtered, and the solvent was evaporated. The crude products were purified by column chromatography and eluted with an ethyl acetate and hexane (3:1) mixture to afford the title compound. To obtain diffraction quality crystals, recrystallization was carried out using an ethyl acetate and hexane (1:1) mixture.

Crystal data

$C_{24}H_{17}N_3O$	$D_x = 1.332$ Mg m^{-3}
$M_r = 363.41$	Mo $K\alpha$ radiation
Monoclinic, $C2/c$	Cell parameters from 9828
$a = 24.0578\ (12)$ Å	reflections
$b = 10.2342\ (5)$ Å	$\theta = 2.5$–$26.6°$
$c = 18.1597\ (9)$ Å	$\mu = 0.08$ mm^{-1}
$\beta = 125.861\ (1)°$	$T = 293\ (2)$ K
$V = 3623.6\ (3)$ Å^3	Block, colourless
$Z = 8$	$0.24 \times 0.22 \times 0.20$ mm

Data collection

Bruker SMART APEX area-detector diffractometer	3677 reflections with $I > 2\sigma(I)$
ω scans	$R_{int} = 0.023$
Absorption correction: none	$\theta_{max} = 28.0°$
20359 measured reflections	$h = -31 \rightarrow 31$
4278 independent reflections	$k = -13 \rightarrow 13$
	$l = -23 \rightarrow 23$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0696P)^2$
$R[F^2 > 2\sigma(F^2)] = 0.050$	$+ 1.847P]$
$wR(F^2) = 0.134$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.05$	$(\Delta/\sigma)_{max} < 0.001$
4278 reflections	$\Delta\rho_{max} = 0.31$ e Å^{-3}
253 parameters	$\Delta\rho_{min} = -0.22$ e Å^{-3}
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

O1—C18	1.217 (2)	C15—C17	1.511 (2)
C7—C17	1.516 (2)		
C16—C15—C17—C24	93.5 (2)	C8—C7—C17—C24	164.3 (1)

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
N1—H1$\cdots$O1^i	0.86	2.08	2.913 (2)	162

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

The H atoms were positioned geometrically and were treated as riding on their parent atoms with C—H distances of 0.93 Å, N—H distances of 0.86 Å and $U_{iso}(H) = 1.2U_{eq}(C,N)$.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics:
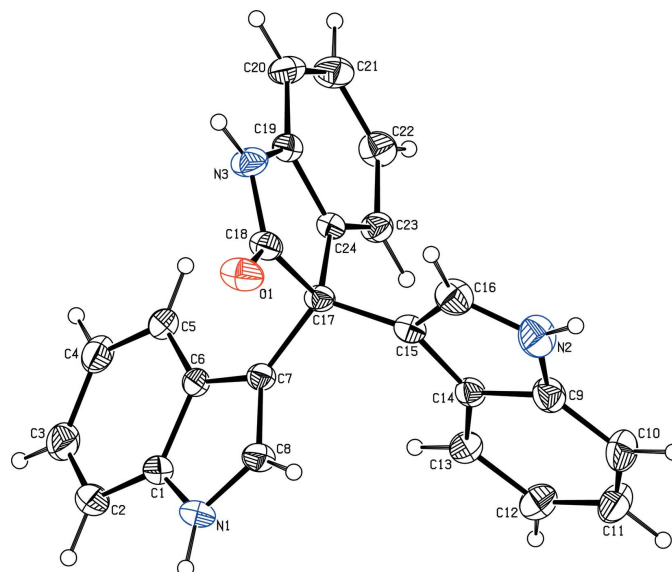

Figure 1
The molecular configuration and atom-numbering scheme for (I). Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii.

ORTEP-3 (Farrugia, 1997) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97* and *PARST* (Nardelli, 1995).

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