

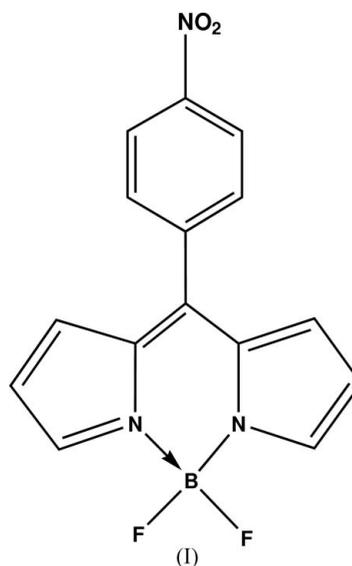
Ai-Jun Cui, Xiao-Jun Peng,\*  
Yun-Ling Gao and Jiang-Li FanState Key Laboratory of Fine Chemicals, Dalian  
University of Technology, 158 Zhongshan Rd,  
Dalian 116012, People's Republic of China

Correspondence e-mail: pengxj@dlut.edu.cn

## Key indicators

Single-crystal X-ray study  
 $T = 293$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.004$  Å  
 $R$  factor = 0.071  
 $wR$  factor = 0.216  
Data-to-parameter ratio = 11.3For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.4,4-Difluoro-8-(4-nitrophenyl)-4-bora-  
3a,4a-diaza-s-indaceneThe molecule of the title compound,  $\text{C}_{15}\text{H}_{10}\text{BF}_2\text{N}_3\text{O}_2$ , is non-planar; the benzene ring is twisted out of the boron-dipyrrromethene mean plane with a dihedral angle of  $57.0$  ( $3$ )°.Received 5 September 2006  
Accepted 20 September 2006

## Comment

Boron-dipyrrromethene (BODIPY) dyes are excellent fluorophores which have attracted a lot of attention with regard to the design of fluorescence labels and biomolecular sensors (Bergström *et al.*, 2002; Trieflinger *et al.*, 2005); investigation of their structures will be helpful in better understanding their photophysical properties (Euler *et al.*, 2002). We recently synthesized a novel BODIPY compound, (I), and determined its crystal structure.As shown in Fig. 1, the BODIPY skeleton formed by three conjugated heterocyclic rings (Table 1) is planar, with an r.m.s. deviation of  $0.0358$  ( $2$ ) Å; the maximum deviation from the mean plane is  $0.0815$  ( $2$ ) Å (atom B1). The dihedral angle between the benzene and BODIPY mean planes is  $57.0$  ( $3$ )°. The F1/B1/F2 plane is nearly perpendicular to the BODIPY plane [dihedral angle =  $89.3$  ( $3$ )°].

## Experimental

Compound (I) was prepared in a one-pot reaction (Kollmannsberger *et al.*, 1998). Pyrrole (4.5 mmol) and *p*-nitrobenzaldehyde (2 mmol) were dissolved in absolute dichloromethane (150 ml) under an argon atmosphere. One drop of trifluoroacetic acid was added and the solution was stirred at room temperature until thin-layer chromatography showed complete consumption of the aldehyde. At this point,

a solution of dichlorodicyanobenzoquinone (2 mmol) in dichloromethane (15 ml) was added and stirring was continued for 10 min, followed by rapid addition of triethylamine (4 ml) and boron trifluoride etherate (4 ml). After stirring for another 2 h, the reaction mixture was washed with water, dried and the solvent evaporated. The residue was chromatographed twice on a silica column [mixture of dichloromethane and hexane (2:1) as eluting solvent]. Recrystallization from ethyl acetate/hexane (3:1) yielded analytically pure samples (yield 30%). Single crystals of (I) were obtained from a hexane–dichloromethane solution (1:3) at 273 K.

Crystal data

$C_{15}H_{10}BF_2N_3O_2$   $V = 684.19 (5) \text{ \AA}^3$   
 $M_r = 313.07$   $Z = 2$   
 Triclinic,  $P\bar{1}$   $D_x = 1.520 \text{ Mg m}^{-3}$   
 $a = 7.8605 (3) \text{ \AA}$  Mo  $K\alpha$  radiation  $\mu = 0.12 \text{ mm}^{-1}$   
 $b = 8.0103 (3) \text{ \AA}$   $T = 293 (2) \text{ K}$   
 $c = 11.4271 (5) \text{ \AA}$  Platelet, red  
 $\alpha = 89.093 (2)^\circ$   $0.20 \times 0.10 \times 0.03 \text{ mm}$   
 $\beta = 85.418 (1)^\circ$   
 $\gamma = 72.554 (1)^\circ$

Data collection

Bruker SMART 1000 CCD area-detector diffractometer 3536 measured reflections  
 $\varphi$  and  $\omega$  scans 2372 independent reflections  
 Absorption correction: multi-scan (SADABS; Sheldrick, 1997) 2185 reflections with  $I > 2\sigma(I)$   
 $R_{int} = 0.034$   
 $\theta_{max} = 25.1^\circ$   
 $T_{min} = 0.978, T_{max} = 0.998$

Refinement

Refinement on  $F^2$   $w = 1/[\sigma^2(F_o^2) + (0.143P)^2 + 0.375P]$   
 $R[F^2 > 2\sigma(F^2)] = 0.071$  where  $P = (F_o^2 + 2F_c^2)/3$   
 $wR(F^2) = 0.216$   $(\Delta/\sigma)_{max} < 0.001$   
 $S = 1.07$   $\Delta\rho_{max} = 0.37 \text{ e \AA}^{-3}$   
 2372 reflections  $\Delta\rho_{min} = -0.37 \text{ e \AA}^{-3}$   
 209 parameters Extinction correction: SHELXL97  
 H-atom parameters constrained Extinction coefficient: 0

Table 1

Selected bond lengths (Å).

F2–B1	1.382 (3)	N1–C1	1.394 (3)
F1–B1	1.379 (3)	N1–B1	1.542 (4)
C8–N2	1.393 (3)	N2–C5	1.339 (4)
C8–C9	1.400 (4)	N2–B1	1.538 (4)
N1–C4	1.336 (4)	C9–C1	1.390 (3)

H atoms were placed in geometrically calculated positions, with C–H = 0.93 Å, and refined in riding mode, with  $U_{iso}(H) = 1.2U_{eq}(C)$ .

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

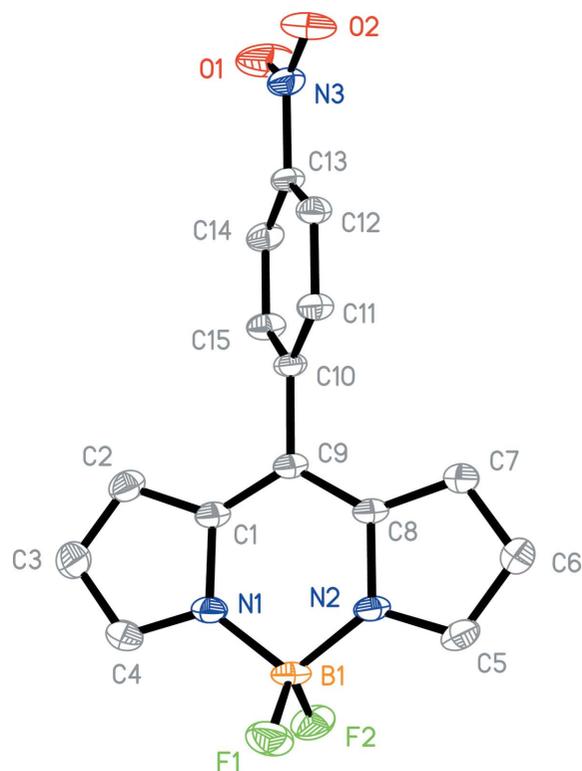


Figure 1

The molecular structure of (I), with 30% probability displacement ellipsoids and H atoms omitted for clarity.

SHELXTL (Bruker, 1997); software used to prepare material for publication: SHELXTL.

This work was financially supported by the Education Ministry of China and the National Natural Science Foundation of China (project Nos. 20128005, 20376010 and 20472012).

References

Bergström, F., Mikhalyov, L., Hägglöf, P., Wortmann, R., Ny, T. & Johansson, L. B. (2002). *J. Am. Chem. Soc.* **124**, 196–204.  
 Bruker (1997). SMART (Version 5.611), SAINT (Version 6.0), SADABS (Version 2.03) and SHELXTL (Version 5.10). Bruker AXS Inc., Madison, Wisconsin, USA.  
 Euler, H., Kirfel, A., Freudenthal, S. J. & Muller, C. E. (2002). *Z. Kristallogr. New Cryst. Struct.* **217**, 541–542.  
 Kollmannsberger, M., Rurack, K., Resch-Genger, U. & Daub, J. (1998). *J. Phys. Chem. A*, **102**, 10211–10220.  
 Sheldrick, G. M. (1997). SHELXL97 and SHELXS97. University of Göttingen, Germany.  
 Trieflinger, C., Rurack, K. & Daub, J. (2005). *Angew. Chem. Int. Ed.* **44**, 2288–2291.