Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

11-(4-Bromophenyl)-10-methyl-8-phenyl-6,8-dihydro-5*H*-benzo[*f*]pyrazolo[3,4-*b*]quinoline

Hugo Serrano,[a] Jairo Quiroga,[a] Justo Cobo,[b] John N. Low[c] and Christopher Glidewell[d]*

[a]Grupo de Investigación de Compuestos Heterocíclicos, Departamento de Química, Universidad de Valle, AA 25360 Cali, Colombia, [b]Departamento de Química Inorgánica y Orgánica, Universidad de Jaén, 23071 Jaén, Spain, [c]Department of Chemistry, University of Aberdeen, Meston Walk, Old Aberdeen AB24 3UE, Scotland, and [d]School of Chemistry, University of St Andrews, Fife KY16 9ST, Scotland

Correspondence e-mail: cg@st-andrews.ac.uk

Received 4 May 2005
Accepted 6 May 2005
Online 14 May 2005

The title compound, $C_{27}H_{20}BrN_3$, is isostructural with the chloro analogue: the molecules are linked by two independent C—H$\cdots\pi$(arene) hydrogen bonds into chains of edge-fused rings.

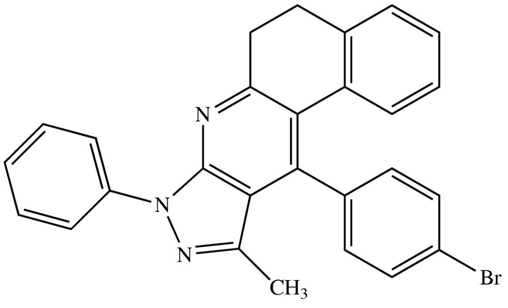
Key indicators

Single-crystal X-ray study
T = 120 K
Mean σ(C–C) = 0.004 Å
R factor = 0.047
wR factor = 0.102
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.

Comment

The title compound, (I) (Fig. 1), is isostructural with 11-(4-chlorophenyl)-10-methyl-8-phenyl-6,8-dihydro-5*H*-benzo[*f*]pyrazolo[3,4-*b*]quinoline, (II) (Serrano *et al.*, 2005).



(I)

The bond lengths and angles, and the molecular conformation, for (I) are all virtually identical with those for (II). Two independent C—H$\cdots\pi$(arene) hydrogen bonds (Table 1) link the molecules of (I) into a [101] chain of centrosymmetric edge-fused rings, just as in (II). There are no direction-specific interactions between adjacent chains: C—H$\cdots$N and C—H$\cdots$Br hydrogen bonds, and aromatic π–π stacking interactions are all absent from the structure of (I).

Experimental

Equimolar amounts of 5-amino-3-methyl-1-phenylpyrazole (173 mg, 1.0 mmol), 2-tetralone (146 mg, 1.0 mmol) and 4-bromobenzaldehyde (185.0 mg, 1.0 mmol) were placed in open Pyrex-glass vessels and irradiated in a domestic microwave oven for 4 min at 600 W. The reaction mixture was then extracted with ethanol, and, after removal of the solvent, the product was recrystallized from ethanol/dimethylformamide to give crystals suitable for single-crystal X-ray diffraction.

Crystal data

$C_{27}H_{20}BrN_3$
M_r = 466.37
Triclinic, $P\overline{1}$
a = 7.0237 (3) Å
b = 12.8964 (7) Å
c = 13.3517 (7) Å
α = 106.630 (3)°
β = 101.423 (3)°
γ = 102.274 (3)°
V = 1088.18 (10) Å^3

Z = 2
D_x = 1.423 Mg m^{-3}
Mo *K*α radiation
Cell parameters from 5001 reflections
θ = 3.1–27.7°
μ = 1.91 mm^{-1}
T = 120 (2) K
Plate, colourless
0.36 × 0.14 × 0.03 mm

Data collection

Bruker–Nonius KappaCCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
$T_{\min} = 0.547$, $T_{\max} = 0.945$
223424 measured reflections

5001 independent reflections
3175 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.085$
$\theta_{\max} = 27.7°$
$h = -8 \rightarrow 9$
$k = -16 \rightarrow 16$
$l = -17 \rightarrow 17$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.102$
$S = 1.03$
5001 reflections
281 parameters

H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0461P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.41$ e Å^{-3}
$\Delta\rho_{\min} = -0.47$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C113—H113···$Cg1^{\rm i}$	0.95	2.71	3.588 (3)	154
C115—H115···$Cg2^{\rm ii}$	0.95	2.81	3.589 (3)	140

Symmetry codes: (i) $-x, 1 - y, -z$; (ii) $1 - x, 1 - y, 1 - z$. Note: $Cg1$ is the centroid of ring C81–C86, and $Cg2$ is the centroid of ring C1,C2,C3,C4,C4*A*,C11*B*

All H atoms were located in difference maps in fully ordered sites; they were then treated as riding atoms, with C—H distances 0.95 (aromatic), 0.98 (methyl) or 0.99 Å (CH_2), and with $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$, or $1.5U_{\rm eq}({\rm C})$ for the methyl group.

Data collection: *COLLECT* (Hooft, 1999); cell refinement: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT*; data reduction: *DENZO* and *COLLECT*; program(s) used to solve structure: *OSCAIL* (McArdle, 2003) and *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *OSCAIL* and *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97* and *PRPKAPPA* (Ferguson, 1999).

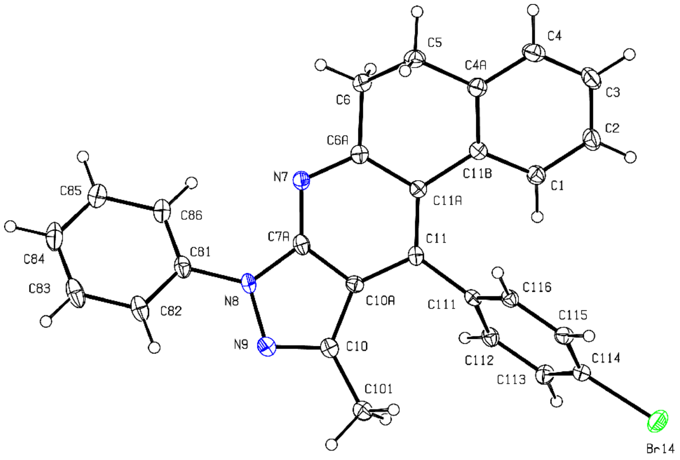


Figure 1
The molecule of compound (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

X-ray data were collected at the EPSRC X-ray Crystallographic Service, University of Southampton, England. JC thanks the Consejería de Innovación, Ciencia y Empresa (Junta de Andalucía, Spain) and the Universidad de Jaén for financial support. JQ and HS thank COLCIENCIAS and UNIVALLE (Universidad del Valle, Colombia) for financial support.

References

Ferguson, G. (1999). *PRPKAPPA*. University of Guelph, Canada.
Hooft, R. W. W. (1999). *COLLECT*. Nonius BV, Delft, The Netherlands.
McArdle, P. (2003). *OSCAIL for Windows*. Version 10. Crystallography Centre, Chemistry Department, NUI Galway, Ireland.
Otwinowski, Z. & Minor, W (1997). *Methods in Enzymology*, Vol. 276, Macromolecular Crystallography, Part A, edited by C. W. Carter Jr and R. M. Sweet, pp. 307–326. New York: Academic Press.
Serrano, H., Quiroga, J., Cobo, J., Low, J. N. & Glidewell, C. (2005). *Acta Cryst.* E**61**, o1058–o1060.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Sheldrick, G. M. (2003). *SADABS*. Version 2.10. University of Göttingen, Germany.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.

Acta Cryst. (2005). E**61**, o1702–o1703 Hugo Serrano *et al.* • $C_{27}H_{20}BrN_3$ **o1703**