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2-(4-Bromophenyl)-1-methyl-1*H*-phenanthro-[9,10-*d*]imidazole

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Key indicators

Single-crystal X-ray study
T = 122 K
Mean σ(C–C) = 0.002 Å
R factor = 0.024
wR factor = 0.057
Data-to-parameter ratio = 22.7

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

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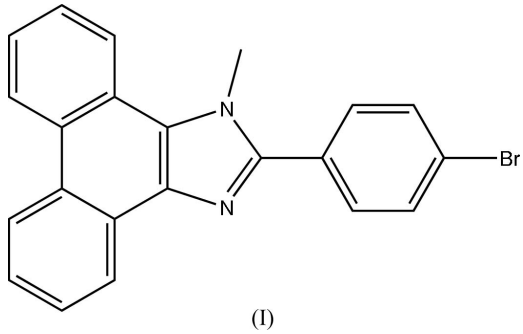
In the title compound, $C_{22}H_{15}BrN_2$, the phenanthrene moiety is slightly skewed. The dihedral angle between the phenanthro[9,10-*d*]imidazole mean plane and the benzene ring is 37.78 (6)°. The crystal packing is stabilized mainly by aromatic interactions, though a weak intermolecular C—H···N hydrogen bond is also observed.

Comment

The title compound, (I) (Fig. 1), was prepared for use as a building block in the syntheses of oligo-phenylene vinylenes for non-linear optical studies. In (I), the imidazole ring is slightly bent from the skewed phenanthrene ring, with atom C16 located 0.092 (2) Å out of the least-squares plane of the phenanthro[9,10-*d*]imidazole system. The dihedral angle between the phenanthro[9,10-*d*]imidazole mean plane and the benzene ring is 37.78 (6)°. This rotation is most probably due to the adjacent *N*-methyl group.



(I)

The crystal packing (Fig. 2) is stabilized mainly by aromatic interactions. A herring-bone pattern is formed by the phenanthrene rings at $y = \frac{1}{4}$ and $\frac{3}{4}$, along with stacking of bromobenzene rings in the planes at $y = 0$ and $\frac{1}{2}$. A weak intermolecular C—H···N hydrogen bond (Table 1) is observed in the crystal structure.

Experimental

The title compound was prepared in accordance with a known procedure (Krebs & Jørgensen, 2001).

Crystal data

$C_{22}H_{15}BrN_2$
M_r = 387.27
Orthorhombic, $Pna2_1$
a = 6.0163 (4) Å
b = 29.332 (3) Å
c = 9.1726 (8) Å
V = 1618.7 (2) Å^3
Z = 4
D_x = 1.589 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 26555 reflections
θ = 2.3–31.0°
μ = 2.55 mm^{-1}
T = 122 (1) K
Plate, pale yellow
0.55 × 0.46 × 0.08 mm

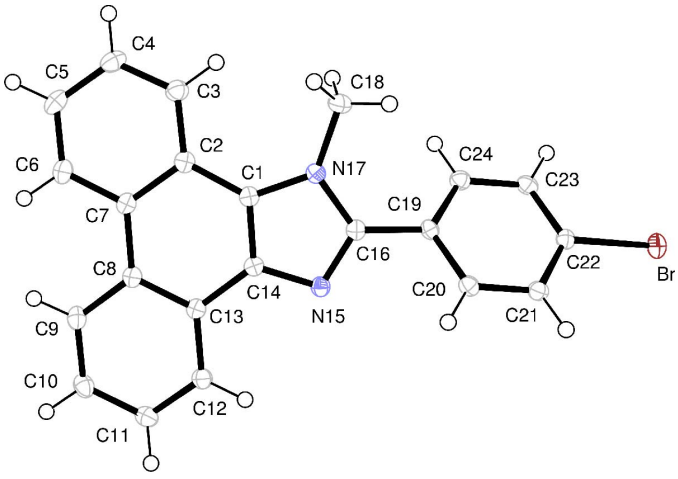


Figure 1
View of (I), with displacement ellipsoids at the 50% probability level. H atoms are shown as spheres of arbitrary radius.

Data collection

Nonius KappaCCD diffractometer	4771 reflections with $I > 2\sigma(I)$
ω and φ scans	$R_{int} = 0.046$
Absorption correction: Gaussian integration (Coppens, 1970)	$\theta_{max} = 31.0°$
$T_{min} = 0.365$, $T_{max} = 0.903$	$h = -8 \rightarrow 8$
36851 measured reflections	$k = -42 \rightarrow 42$
5137 independent reflections	$l = -13 \rightarrow 13$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0299P)^2 + 0.9474P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.024$	$(\Delta/\sigma)_{max} = 0.001$
$wR(F^2) = 0.057$	$\Delta\rho_{max} = 0.45$ e Å^{-3}
$S = 1.15$	$\Delta\rho_{min} = -0.34$ e Å^{-3}
5137 reflections	Absolute structure: Flack (1983), 2414 Friedel reflections
226 parameters	Flack parameter = −0.009 (6)
H-atom parameters constrained	

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

D—H···A	D—H	H···A	D···A	D—H···A
C23—H23···N15^{i}	0.95	2.54	3.419 (2)	154

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

All H atoms were located in a difference Fourier map and refined using a riding model, with fixed individual displacement parameters set at 1.2–1.5 times U_{eq} of the parent atom (C—H = 0.95–0.98 Å).

Data collection: *COLLECT* (Nonius, 1999); cell refinement: *DIRAX* (Duisenberg, 1992); data reduction: *EvalCCD* (Duisenberg *et al.*, 2003); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996); software used to prepare material for publication: *SHELXL97*.

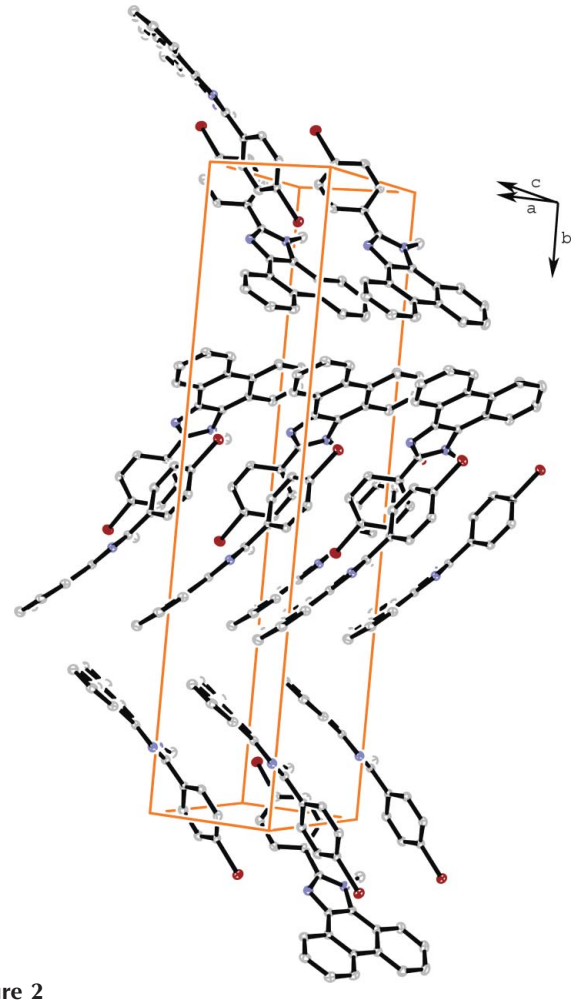


Figure 2
The crystal packing of (I). H atoms have been omitted for clarity.

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