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)$^\circ$. 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)$^\circ$. This rotation is most probably due to the adjacent N-methyl group.

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 \(\frac{1}{4}\). 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, \(Pna\_2_1\)

\(a = 6.0163\) (4) Å

\(b = 29.332\) (3) Å

\(c = 9.1726\) (8) Å

\(V = 1618.7\) (2) Å$^3$

\(Z = 4\)

\(D_\text{r} = 1.589\) Mg m$^{-3}$

Mo \(K\alpha\) radiation

Cell parameters from 26555 reflections

\(\theta = 2.3\text{ to }31.0^\circ\)

\(\mu = 2.55\) mm$^{-1}$

\(T = 122\) (1) K

Plate, pale yellow

0.55 × 0.46 × 0.08 mm

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Data collection
Nonius KappaCCD diffractometer
ω and ψ scans
Absorption correction: Gaussian integration (Coppens, 1970)

$T_{\text{min}} = 0.365, T_{\text{max}} = 0.903$
36851 measured reflections
5137 independent reflections
4771 reflections with $I > 2\sigma(I)$

Refinement
Refinement on $F^2$

$wR(F^2) = 0.057$
$S = 1.15$
5137 reflections
226 parameters
H-atom parameters constrained

$w = 1/\left[\sigma^2(F_o^2) + (0.0299 P)^2 + 0.9474 P\right]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta\sigma/\sigma)_{\text{max}} = 0.001$  
$\Delta\rho_{\text{max}} = 0.45 e \text{Å}^{-3}$  
$\Delta\rho_{\text{min}} = -0.34 e \text{Å}^{-3}$

Absolute structure: Flack (1983), 2414 Friedel reflections  
Flack parameter = −0.009 (6)

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

<table>
<thead>
<tr>
<th>D—H···A</th>
<th>D—H</th>
<th>H···A</th>
<th>D···A</th>
<th>D—H···A</th>
</tr>
</thead>
<tbody>
<tr>
<td>C23—H23···N15'</td>
<td>0.95</td>
<td>2.54</td>
<td>3.419 (2)</td>
<td>154</td>
</tr>
</tbody>
</table>

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

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

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References