

2-Amino-4-phenyl-5,6-dihydrobenzo-*[h]*quinoline-3-carbonitrile–3-amino-1-phenyl-9,10-dihydrophenanthrene-2,4-dicarbonitrile (5/3)

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Received 11 September 2011; accepted 3 October 2011

Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; disorder in main residue; R factor = 0.040; wR factor = 0.119; data-to-parameter ratio = 7.5.

The asymmetric unit of the 5:3 title co-crystal of 2-amino-4-phenyl-5,6-dihydrobenzo[*h*]quinoline-3-carbonitrile and 3-amino-1-phenyl-9,10-dihydrophenanthrene-2,4-dicarbonitrile, $0.625\text{C}_{20}\text{H}_{15}\text{N}_3 \cdot 0.375\text{C}_{22}\text{H}_{15}\text{N}_3$, has the atoms of the fused-ring system and those of the amino, cyano and phenyl substituents overlapped. The fused-ring system is buckled owing to the ethylene linkage in the central ring, the two flanking aromatic rings being twisted by $20.1(1)^\circ$. This ethylene portion is disordered over two positions in a 1:1 ratio. The phenyl ring is twisted by $69.5(1)^\circ$ relative to the amino- and cyano-bearing aromatic ring. In the crystal, two molecules are linked by an $\text{N}-\text{H} \cdots \text{N}$ hydrogen bond, generating a helical chain along [010].

Related literature

For the synthesis, see: Aly *et al.* (1991); Paul *et al.* (1998). For related structures, see: Asiri *et al.* (2011*a,b*).



Experimental

Crystal data

$0.625\text{C}_{20}\text{H}_{15}\text{N}_3 \cdot 0.375\text{C}_{22}\text{H}_{15}\text{N}_3$ $V = 1535.47(6) \text{ \AA}^3$
 $M_r = 306.36$ $Z = 4$
 Orthorhombic, $P2_12_12_1$ $\text{Cu K}\alpha$ radiation
 $a = 6.9611(2) \text{ \AA}$ $\mu = 0.62 \text{ mm}^{-1}$
 $b = 12.6093(2) \text{ \AA}$ $T = 100 \text{ K}$
 $c = 17.4933(3) \text{ \AA}$ $0.30 \times 0.20 \times 0.02 \text{ mm}$

Data collection

Agilent SuperNova Dual 6293 measured reflections
 diffractometer with an Atlas 1794 independent reflections
 detector 1707 reflections with $I > 2\sigma(I)$
 Absorption correction: multi-scan $R_{\text{int}} = 0.018$
 (*CrysAlis PRO*; Agilent, 2010)
 $T_{\text{min}} = 0.835$, $T_{\text{max}} = 0.988$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.040$ H atoms treated by a mixture of
 $wR(F^2) = 0.119$ independent and constrained
 $S = 1.05$ refinement
 1794 reflections $\Delta\rho_{\text{max}} = 0.19 \text{ e \AA}^{-3}$
 240 parameters $\Delta\rho_{\text{min}} = -0.23 \text{ e \AA}^{-3}$
 24 restraints

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H} \cdots A$	$D-\text{H}$	$\text{H} \cdots A$	$D \cdots A$	$D-\text{H} \cdots A$
$\text{N2}-\text{H1} \cdots \text{N3}^i$	0.88 (1)	2.37 (2)	3.175 (2)	152 (3)

Symmetry code: (i) $-x + 2, y + \frac{1}{2}, -z + \frac{5}{2}$.

Data collection: *CrysAlis PRO* (Agilent, 2010); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

We thank King Abdulaziz University and the University of Malaya for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZS2145).

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