

3-Amino-1-methyl-9,10-dihydro-phenanthrene-2,4-dicarbonitrile

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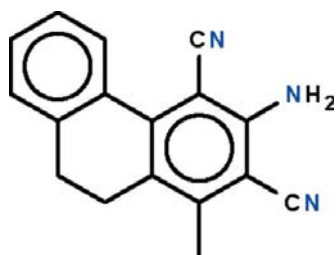
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Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.034; wR factor = 0.091; data-to-parameter ratio = 7.4.

The asymmetric unit of the title compound, $\text{C}_{17}\text{H}_{13}\text{N}_3$, contains two independent molecules, which are non-planar as they are buckled owing to the ethylene portion. The dihedral angle between the benzene rings is $26.4(1)^\circ$ in one molecule and $32.9(1)^\circ$ in the other. In the crystal, the molecules are disposed about a false inversion center, and are linked by two $\text{N}-\text{H}\cdots\text{N}$ hydrogen bonds, generating a dimer. The dimers are linked by further $\text{N}-\text{H}\cdots\text{N}$ hydrogen bonds, resulting in a chain that runs along the longest axis of the orthorhombic unit cell.

Related literature

For the synthesis of dihydrophenanthrenes, see: Dellagrega *et al.* (2000); Ram & Goel (1997).



Experimental

Crystal data

$\text{C}_{17}\text{H}_{13}\text{N}_3$	$V = 2652.78(12) \text{ \AA}^3$
$M_r = 259.30$	$Z = 8$
Orthorhombic, $Pna2_1$	Cu $K\alpha$ radiation
$a = 26.8587(7) \text{ \AA}$	$\mu = 0.62 \text{ mm}^{-1}$
$b = 8.8158(2) \text{ \AA}$	$T = 100 \text{ K}$
$c = 11.2035(3) \text{ \AA}$	$0.30 \times 0.20 \times 0.02 \text{ mm}$

Data collection

Agilent SuperNova Dual diffractometer with an Atlas detector	10819 measured reflections
Absorption correction: multi-scan (<i>CrysAlis PRO</i> ; Agilent, 2010)	2800 independent reflections
$T_{\min} = 0.836$, $T_{\max} = 0.988$	2621 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.033$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.034$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.091$	$\Delta\rho_{\max} = 0.16 \text{ e \AA}^{-3}$
$S = 1.09$	$\Delta\rho_{\min} = -0.20 \text{ e \AA}^{-3}$
2800 reflections	
379 parameters	
1 restraint	

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N2}-\text{H21}\cdots\text{N4}$	0.91 (4)	2.15 (4)	3.007 (3)	156 (3)
$\text{N2}-\text{H22}\cdots\text{N6}^i$	0.91 (3)	2.38 (3)	3.265 (3)	164 (2)
$\text{N5}-\text{H51}\cdots\text{N1}^{ii}$	0.91 (4)	2.12 (4)	3.012 (3)	168 (3)
$\text{N5}-\text{H52}\cdots\text{N3}$	0.91 (3)	2.41 (3)	3.283 (3)	161 (3)

Symmetry codes: (i) $x, y, z + 1$; (ii) $x, y, z - 1$.

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).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5310).

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