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3-Amino-1-methyl-9,10-dihydrophenanthrene-2,4-dicarbonitrile

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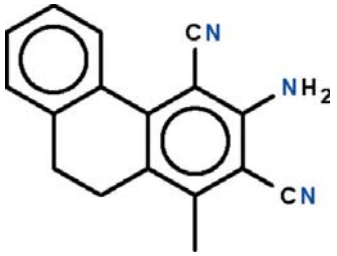
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.003 Å; R factor = 0.034; wR factor = 0.091; data-to-parameter ratio = 7.4.

The asymmetric unit of the title compound, $C_{17}H_{13}N_3$, 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)° in one molecule and 32.9 (1)° in the other. In the crystal, the molecules are disposed about a false inversion center, and are linked by two N—H···N hydrogen bonds, generating a dimer. The dimers are linked by further N—H···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: Dellagreca *et al.* (2000); Ram & Goel (1997).



Experimental

Crystal data

$C_{17}H_{13}N_3$
M_r = 259.30
Orthorhombic, $Pna2_1$
a = 26.8587 (7) Å
b = 8.8158 (2) Å
c = 11.2035 (3) Å
V = 2652.78 (12) Å^3
Z = 8
Cu $K\alpha$ radiation
μ = 0.62 mm^{-1}
T = 100 K
0.30 × 0.20 × 0.02 mm

Data collection

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

Refinement

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

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H21···N4	0.91 (4)	2.15 (4)	3.007 (3)	156 (3)
N2—H22···N6^{i}	0.91 (3)	2.38 (3)	3.265 (3)	164 (2)
N5—H51···N1^{ii}	0.91 (4)	2.12 (4)	3.012 (3)	168 (3)
N5—H52···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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