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An orthorhombic polymorph of naphthalene-2,3-dicarbonitrile

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Key indicators

Single-crystal X-ray study
T = 153 K
Mean σ(C–C) = 0.003 Å
R factor = 0.037
wR factor = 0.105
Data-to-parameter ratio = 7.0

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

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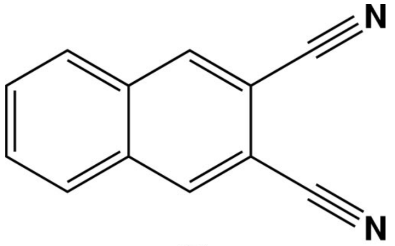
The achiral title compound, $C_{12}H_6N_2$, crystallizes in the non-centrosymmetric space group $P2_12_12_1$. Its structure is compared with that of the triclinic polymorph, which crystallizes with two independent molecules in space group *P*1. In the crystal structure, the molecules stack along the *a* direction, and zigzag chains, extending in the *b* direction, are formed owing to the presence of C—H···N intermolecular contacts.

Comment

Crystals of the title compound, (I), the orthorhombic polymorph of 2,3-dicyanonaphthalene, were obtained by slow evaporation of a $CDCl_3$ solution. The molecular structure of (I) is shown in Fig. 1. The crystal structure of the triclinic polymorph, (II), obtained by sublimation, has been reported by Janczak & Kubiak (2000). That structure was refined in the non-centrosymmetric space group *P*1, with two independent molecules in the unit cell.



(I)

In the napthalene nucleus of (I), the C2—C3 and C9—C10 bonds are long [1.432 (2) and 1.423 (3) Å, respectively], while the C1—C2, C3—C4, C5—C6 and C7—C8 bonds are short, ranging from 1.365 (3) to 1.373 (2) Å. The remainder of the bonds, C1—C9, C4—C10, C5—C10, C6—C7 and C8—C9, have an intermediate length, ranging from 1.406 (3) to 1.418 (3) Å. This variation indicates that the π electrons are not fully delocalized over the whole nucleus of the naphthalene ring. This situation is similar to that observed in (II) (Janczak & Kubiak, 2000). The naphthalene ring is planar, with a maximum deviation of 0.008 (2) Å for atom C8. The deviations of the cyano N atoms from this plane are −0.046 (2) Å for atom N1 and 0.071 (2) Å for atom N2.

In the crystal structure, the molecules stack in the *a* direction, and zigzag chains, extending in the *b* direction, are built up owing to the presence of C—H···N intermolecular contacts (Fig. 2 and Table 1). The H···N distances [2.57 (2) and 2.63 (2) Å; see Table 1 for details] are shorter than those observed in (II) [*cf.* 2.702 (5) and 2.741 (5) Å], in which the chains are more nearly linear.

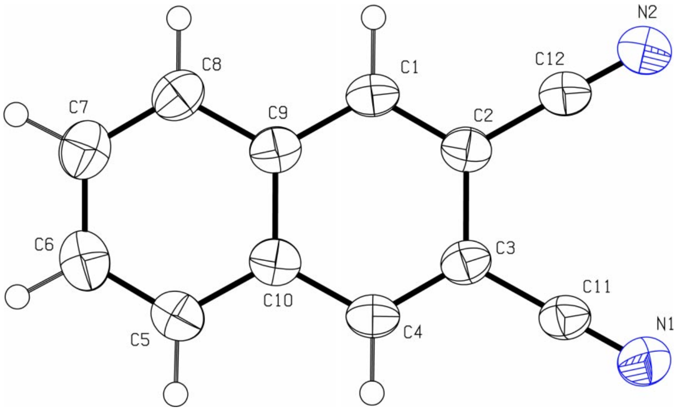


Figure 1
The molecular structure of (I), showing the atomic numbering scheme and displacement ellipsoids at the 50% probability level.

Experimental

Colourless block-like crystals of 2,3-dicyanonaphthalene (Acros Organics, Belgium) were obtained by slow evaporation of a solution of (I) in $CDCl_3$ in an NMR tube.

Crystal data

$C_{12}H_6N_2$
$M_r = 178.19$
Orthorhombic, $P2_12_12_1$
$a = 3.8144\ (5)$ Å
$b = 12.175\ (2)$ Å
$c = 18.806\ (3)$ Å
$V = 873.4\ (2)$ Å^3
$Z = 4$
$D_x = 1.355$ Mg m^{-3}

Mo $K\alpha$ radiation
Cell parameters from 6447 reflections
$\theta = 1.7$–$26.1°$
$\mu = 0.08$ mm^{-1}
$T = 153\ (2)$ K
Block, colourless
$0.45 \times 0.25 \times 0.15$ mm

Data collection

Stoe IPDS-II diffractometer
ω scans
Absorption correction: none
6296 measured reflections
1054 independent reflections
915 reflections with $I > 2\sigma(I)$

$R_{\rm int} = 0.066$
$\theta_{\rm max} = 26.1°$
$h = -4 \rightarrow 4$
$k = -15 \rightarrow 15$
$l = -23 \rightarrow 21$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.037$
$wR(F^2) = 0.105$
$S = 0.87$
1054 reflections
151 parameters
All H-atom parameters refined

$w1/[\sigma^2(F_o^2) + (0.0678P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max} = 0.12$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.14$ e Å^{-3}
Extinction correction: none

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

	D—H	H···A	D···A	D—H···A
C1—H1···N1$^{\rm i}$	0.99 (2)	2.57 (2)	3.487 (2)	154.7 (16)
C4—H4···N2$^{\rm ii}$	0.97 (2)	2.63 (2)	3.496 (3)	148.6 (16)

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

In the absence of significant anomalous dispersion effects, Friedel pairs were merged and the $\Delta f''$ term set to zero. H atoms were located in difference Fourier maps and refined isotropically [C—H = 0.97 (2)–1.00 (2) Å].

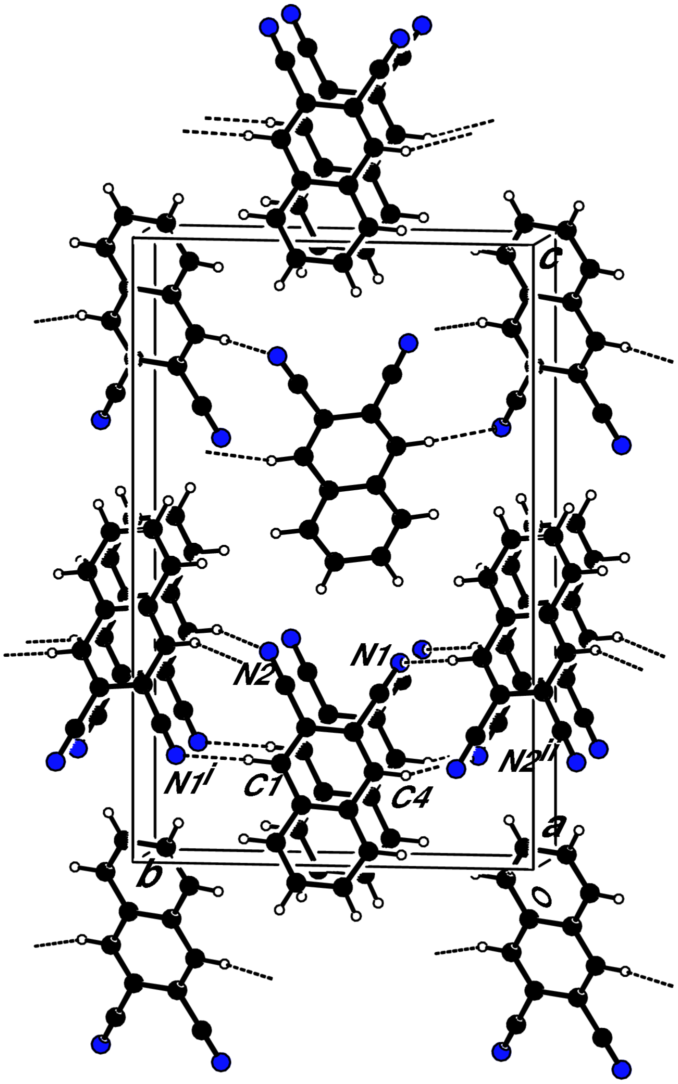


Figure 2
The crystal packing in (I), viewed down the a axis. The C—H···N hydrogen bonds are shown as dashed lines. The symmetry operations correspond to those given in Table 1.

Data collection: *X-AREA* (Stoe & Cie, 2004); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

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