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4,7-Phenanthroline

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The structure of 4,7-phenanthroline, $C_{12}H_8N_2$, has been determined at 180 K. The molecular unit possesses pseudo-C_{2v} point symmetry but does not possess crystallographic mirror symmetry. The molecules form stacks approximately along the *b* direction, with molecules in adjacent stacks forming an interplane angle of *ca* 54°.

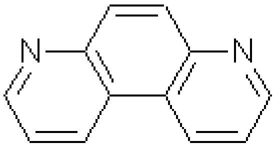
Key indicators

Single-crystal X-ray study
T = 180 K
Mean σ(C–C) = 0.007 Å
R factor = 0.063
wR factor = 0.161
Data-to-parameter ratio = 8.7

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

Comment

As part of a continuing study of cocrystal formation between organic acids and N-containing organic bases, we have determined the structure of 4,7-phenanthroline, (I), at 180 K. The molecular unit possesses pseudo-C_{2v} point symmetry, but does not exhibit crystallographic mirror symmetry. Similar observations have been made for the isomeric 1,10-phenanthroline (Nishigaki *et al.*, 1978). In the crystal structure, 4,7-phenanthroline forms planar stacks approximately along the *b* direction with molecules in adjacent stacks forming an interplane angle of *ca* 54° (Fig. 2); this contrasts with the observation of two approximately perpendicular layers in 1,10-phenanthroline. There is no conclusive evidence for directional C—H···N contacts in 4,7-phenanthroline, with the shortest H···N contacts, $H1\cdots N7^{i} = 2.72$, $H8\cdots N4^{ii} = 3.00$ and $H10\cdots N7^{iii} = 3.00$ Å, exhibiting C—H···N angles of 153.6, 128.6 and 119.5°, respectively [symmetry codes: (i) $\frac{3}{2} - x, -1 + y, \frac{1}{2} + z$; (ii) $\frac{1}{2} + x, 1 - y, z$; (iii) $\frac{3}{2} - x, y, \frac{1}{2} + z$].



(I)

Experimental

4,7–Phenanthroline was obtained from Aldrich and recrystallized from ethanol.

Crystal data

$C_{12}H_8N_2$
M_r = 180.20
Orthorhombic, $Pca2_1$
a = 19.141 (4) Å
b = 3.8417 (4) Å
c = 11.564 (2) Å
V = 850.4 (3) Å^3
Z = 4
D_x = 1.408 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 6723 reflections
θ = 1.0–25.0°
μ = 0.09 mm^{-1}
T = 180 (2) K
Plate, colourless
0.30 × 0.09 × 0.05 mm

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Data collection

Nonius KappaCCD diffractometer
Thin-slice ω and φ scans
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995)
$T_{\min} = 0.975$, $T_{\max} = 0.996$
2186 measured reflections
1099 independent reflections
812 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.080$
$\theta_{\max} = 25.1°$
$h = -22 \rightarrow 17$
$k = -4 \rightarrow 3$
$l = -13 \rightarrow 10$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.063$
$wR(F^2) = 0.161$
$S = 1.09$
1099 reflections
127 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.078P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.002$
$\Delta\rho_{\max} = 0.30$ e Å^{-3}
$\Delta\rho_{\min} = -0.27$ e Å^{-3}
Absolute structure: Flack (1983)
Flack parameter = −3 (8)

The absolute structure was not determined. Friedel opposites merged prior to merging of data in $Pca2_1$. H atoms were placed geometrically and allowed to ride during subsequent refinement with an isotropic displacement parameter fixed at 1.2 times $U_{\rm iso}$ for the C atom to which they are attached.

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *HKL SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *HKL DENZO* and *SCALEPACK* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *XP* (Sheldrick, 1993); software used to prepare material for publication: *SHELXL*97.

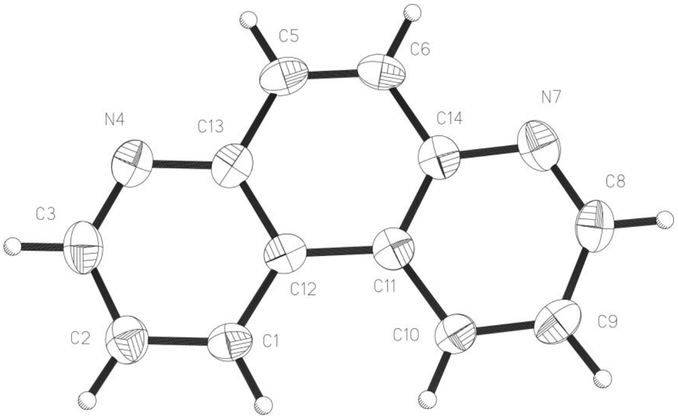

Figure 1
The molecular unit of the title compound showing displacement ellipsoids at the 50% probability level.

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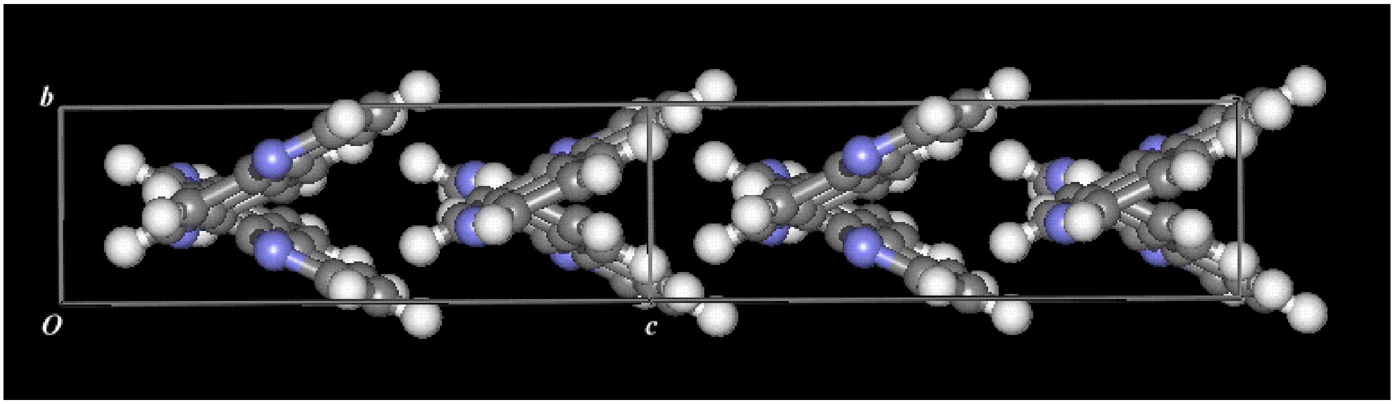

Figure 2
Projection onto (100) showing molecular stacks tilted with respect to each other with molecules in adjacent stacks forming an interplane angle of *ca* 54°.