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Dimorphism of 2,2′:6′,2″:6″,2‴-quaterpyridine

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The title compound, $C_{20}H_{14}N_4$, shows dimorphism, with crystals obtained from different solvents displaying different crystal structures. The main structural difference between the two polymorphs concerns the crystal packing, the dihedral angle between two nearly planar molecules being distinctly different. In the polymorph reported here, the molecule lies on an inversion centre.

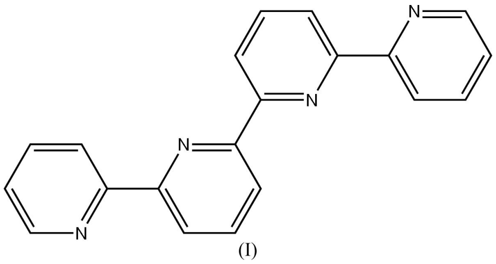
Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.002 Å
R factor = 0.076
wR factor = 0.246
Data-to-parameter ratio = 22.6

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

Comment

Polymorphism occurs frequently in crystal chemistry (Mitscherlich, 1822) and has been extensively described in the literature (*e.g.* Dunitz, 1979; Glusker, 1994). In the case of 2,2′:6′,2″:6″,2‴-quaterpyridine, (I), two polymorphs, *viz.* (I*a*) and (I*b*), were obtained by crystallization from different solvents. Polymorph (I*a*) was obtained by slow evaporation of an acetonitrile solution, while polymorph (I*b*) was obtained by evaporation of a toluene solution; the crystal structure of the latter was solved and described by Constable *et al.* (1990). Polymorphs (I*a*) and (I*b*) both crystallize in the monoclinic crystal system in space groups *C*2/*c* and $P2_1/n$, respectively. The Niggli values (Spek, 2003; Table 1) demonstrate clearly that the reduced cells are different.



(I)

The main structural difference between (I*a*) and (I*b*) concerns the packing of the molecules (Fig. 2 and Fig. 3). Each structure contains two sets of molecules; each set is composed of molecules that are parallel to each other. The dihedral angles between the two sets are 49.65 (16) and 35.65 (19)° for (I*a*) and (I*b*), respectively; only non-H atoms were used for the least-squares-plane calculations. The largest deviation from planarity within a molecule in (I*a*) is 0.109 Å (r.m.s. deviation 0.0136 Å), whereas this is slightly larger in (I*b*), at 0.169 Å (r.m.s. deviation 0.0211 Å). The two polymorphs have crystallographic inversion symmetry.

Experimental

Crystals of (I*a*) were obtained from a reaction mixture of (I*a*) and 2*H*-pyran-2-one in acetonitrile. After the discovery that (I*a*) was a polymorph of (I*b*), the cell parameters of pure (I*a*) from acetonitrile

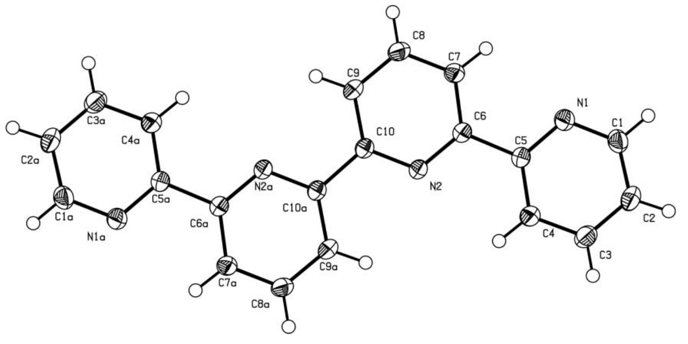


Figure 1
The molecular structure of (I*a*), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii. Atoms labelled with the suffix a are at the symmetry position ($\frac{3}{2} - x, \frac{1}{2} - y, 1 - z$).

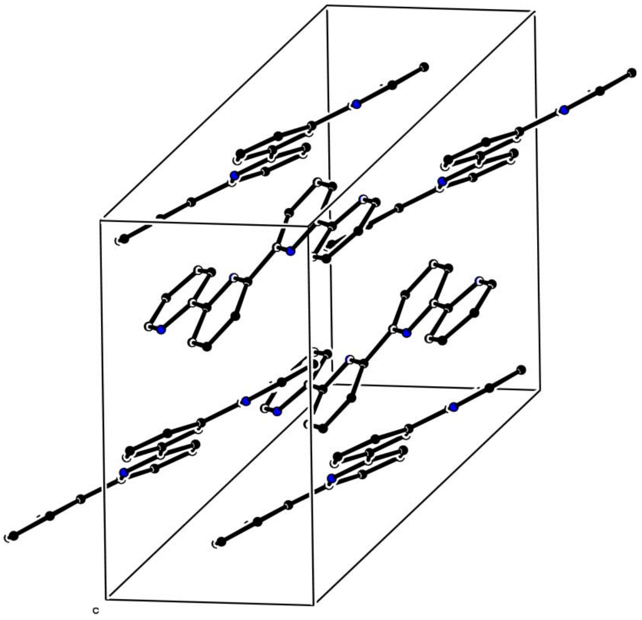


Figure 2
A packing diagram of (I*a*). H atoms have been omitted.

were checked to be identical with those found for the first crystal of (I*a*).

Crystal data

$C_{20}H_{14}N_4$
M_r = 310.35
Monoclinic, $C2/c$
a = 15.327 (2) Å
b = 12.436 (2) Å
c = 8.543 (2) Å
β = 113.50 (2)°
V = 1493.3 (5) Å^3
Z = 4

D_x = 1.381 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2162 reflections
θ = 2.8–26.9°
μ = 0.09 mm^{-1}
T = 173 (2) K
Plate, colourless
0.55 × 0.40 × 0.12 mm

Data collection

Oxford Diffraction XCALIBUR diffractometer
ω scans
11056 measured reflections
2465 independent reflections
1565 reflections with $I > 2\sigma(I)$

$R_{\rm int}$ = 0.088
$\theta_{\rm max}$ = 32.2°
$h = -22 \rightarrow 22$
$k = -18 \rightarrow 18$
$l = -12 \rightarrow 11$

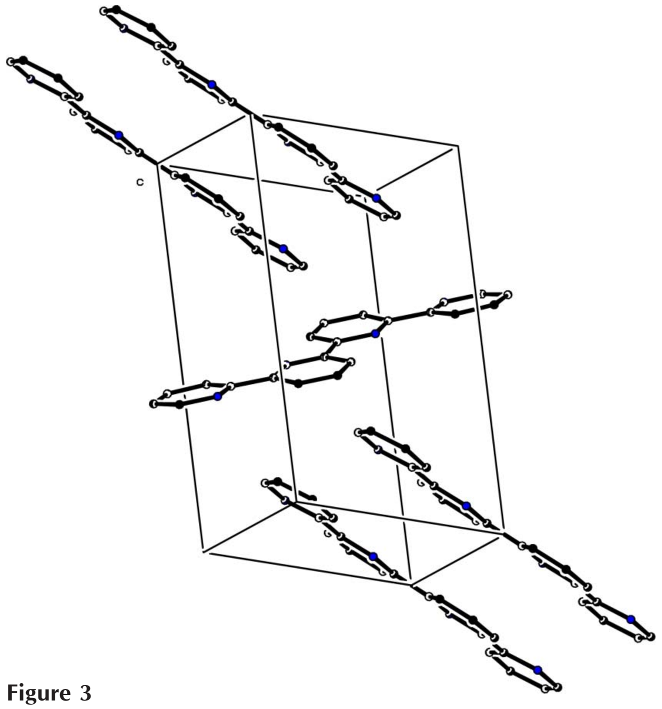


Figure 3
A packing diagram of (I*b*). H atoms have been omitted.

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.076
$wR(F^2)$ = 0.246
S = 1.14
2465 reflections
109 parameters

H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.111P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max}$ = 0.37 e Å^{-3}
$\Delta\rho_{\rm min}$ = −0.35 e Å^{-3}

Table 1
Comparative table of reduced (Niggli) cell parameters (Å^2) of polymorphs (I*a*) and (I*b*).

Polymorph	*a.a*	*b.b*	*c.c*	*b.c*	*a.c*	*a.b*
(I*a*)	72.983	97.393	97.393	20.066	26.105	26.106
(I*b*)	40.297	66.896	221.831	0.000	−16.662	0.000

All H atoms were located by difference Fourier synthesis and refined with fixed individual displacement parameters [$U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C)], using a riding model with aromatic C—H = 0.95 Å.

Data collection: *CrysAlisCCD* (Oxford Diffraction, 2005); cell refinement: *CrysAlisRED* (Oxford Diffraction, 2005); data reduction: *CrysAlisRED*; 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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