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5,6-Bis(2-pyridyl)-2,3-pyrazinedicarbonitrile

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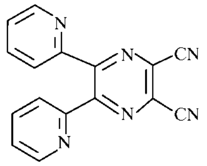
The crystal structure of the title compound, $C_{16}H_8N_6$, contains two independent molecules with no significant difference in their structures. The pyrazine ring makes dihedral angles of 36.7 (2) and 36.5 (3)° with the two pyridine rings in one molecule, and 43.1 (2) and 38.4 (1)° in the other. The dihedral angles between the two pyridine rings are 58.2 (2) and 56.0 (2)°, respectively. The favoured orientation of the pyridine rings is such that their N atoms face each other.

Comment

Bridging polypyridyl compounds have attracted much interest as building blocks for supramolecular assemblies (Scandola *et al.*, 1992; Scott *et al.*, 1999). Some of the polypyridyl ligands have been actively studied in recent years because of the potential functionality of their metal complexes as molecular devices (Nallas & Brewer, 1997; Brauns *et al.*, 1997) and DNA probes (Yam *et al.*, 1995; Holmlin *et al.*, 1999). In the present paper, we report the synthesis and crystal structure of a new polypyridyl compound, namely 5,6-bis(2-pyridyl)-2,3-pyrazinedicarbonitrile, (I).



(I)

The title compound consists of a pyrazine ring substituted with two pyridine rings and two nitrile groups. The unit cell contains two symmetry-independent molecules with no significant difference in their structures (Fig. 1). The two pyridine rings are not coplanar with each other or with the pyrazine ring due to steric clashes between the H atoms in the pyridyl rings. The torsion angles between the carbon–carbon bonds connecting the pyridine rings to the pyrazine ring (C7—C5—C6—C12 and C23—C21—C22—C28) are 18.8 (3) and 20.0 (4)° for the two molecules, respectively. In the pyrazine rings, the maximum deviations of any atom from the best-fit planes describing them are 0.0663 (2) and 0.0707 (1) Å. The pyrazine rings make dihedral angles of 36.7 (2) and 36.5 (3)° with the two pyridine rings in one molecule, and 43.1 (2) and 38.4 (1)° in the other. The dihedral angles of the pyridine rings are 58.2 (2) and 56.0 (2)°, and their N atoms face each other. These distortions from planarity in the title molecule are similar to its analogues (Rasmussen *et al.*, 1990). Both nitriles in each molecule are equivalent and typical of N≡C triple bonds. The other C—N bond distances lie in the range 1.329 (5)–1.352 (4) Å. The bond angles of C2—C1—N1, C18—C17—N7, C4—C3—N2 and C20—C19—N8 are close to 180°. There are no hydrogen bonds or π–π stacking interactions between the different molecules.

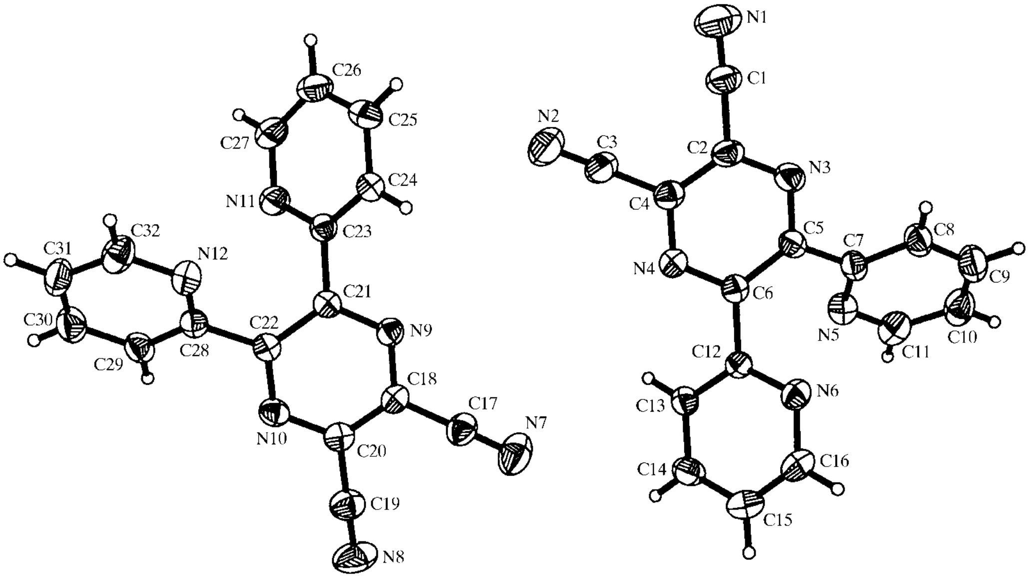


Figure 1
The molecular structure of (I) showing 30% probability displacement ellipsoids.

Experimental

The title compound was synthesized by stirring a 1:1 molar ratio of 2,2′-pyridine (0.43 g, 2.0 mmol) and diaminomaleonitrile (0.22 g, 2.0 mmol) in the presence of several drops of acetic acid in ethanol solution (50 ml) under an argon atmosphere at reflux for *ca* 6 h. The solvent was concentrated *in vacuo* to afford a colourless solid which was purified by recrystallization from CH_2Cl_2/CH_3OH to obtain single crystals suitable for X-ray diffraction. The title compound is unstable when exposed to air for a period of several months.

Crystal data

$C_{16}H_8N_6$
$M_r = 284.28$
Orthorhombic, $Pna2_1$
$a = 16.996$ (2) Å
$b = 8.1356$ (11) Å
$c = 20.660$ (3) Å
$V = 2856.8$ (7) Å^3
$Z = 8$
$D_x = 1.322$ Mg m^{-3}

Mo $K\alpha$ radiation
Cell parameters from 10162 reflections
$\theta = 1.97$–25.03°
$\mu = 0.086$ mm^{-1}
$T = 298$ (2) K
Prism, colourless
0.30 × 0.25 × 0.20 mm

Data collection

Bruker SMART 1000 diffractometer
ω scans
Absorption correction: multi-scan [*SAINT* (Bruker, 1998) and *SADABS* (Sheldrick, 1997)]
$T_{min} = 0.975$, $T_{max} = 0.983$
11285 measured reflections

3743 independent reflections
2589 reflections with $I > 2\sigma(I)$
$R_{int} = 0.037$
$\theta_{max} = 25.03°$
$h = -17 \rightarrow 20$
$k = -9 \rightarrow 9$
$l = -15 \rightarrow 24$
Intensity decay: <1%

Table 1
Selected geometric parameters (Å, °).

N1—C1	1.143 (6)	C17—N7	1.137 (4)
N2—C3	1.140 (4)	C18—N9	1.335 (4)
N3—C2	1.340 (4)	C19—N8	1.140 (5)
N3—C5	1.340 (4)	C20—N10	1.346 (4)
N4—C6	1.333 (3)	C21—N9	1.335 (4)
N4—C4	1.342 (4)	C22—N10	1.330 (4)
C2—N3—C5	117.5 (3)	N7—C17—C18	178.9 (4)
C6—N4—C4	118.1 (3)	N8—C19—C20	178.4 (4)
N1—C1—C2	177.5 (5)	C18—N9—C21	117.4 (3)
N2—C3—C4	178.6 (4)	C22—N10—C20	117.2 (2)

Refinement

Refinement on F^2
$R(F) = 0.037$
$wR(F^2) = 0.101$
$S = 0.983$
3743 reflections
398 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0552P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.003$
$\Delta\rho_{max} = 0.13$ e Å^{-3}
$\Delta\rho_{min} = -0.13$ e Å^{-3}
Extinction correction: *SHELXL*97 (Sheldrick, 1997)
Extinction coefficient: 0.0062 (6)

H atoms were located by geometry but their parameters were not refined.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *XP* (Sheldrick, 1997).

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: VJ1118). Services for accessing these data are described at the back of the journal.

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