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Structure of 2,3-Bis(2-pyridyl)pyrazine

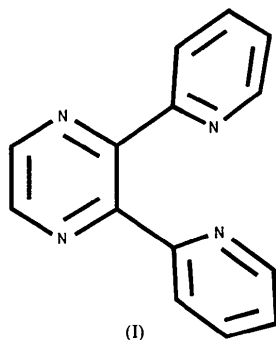
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(Received 14 January 1991; accepted 27 February 1991)

Abstract. $C_{14}H_{10}N_4$ (dpp), $M_r = 234.26$, orthorhombic, $Pbcn$, $a = 16.439$ (3), $b = 9.448$ (2), $c = 7.478$ (2) Å, $V = 1161.5$ (3) Å³, $Z = 4$, $D_x = 1.34$ g cm⁻³, graphite-monochromated Mo $K\alpha$, $\lambda = 0.71073$ Å, $\mu = 0.8$ cm⁻¹, $F(000) = 488$, $T = 294$ (1) K, $R = 0.048$ for 630 observed reflections. The molecule has crystallographic twofold rotational symmetry. The rotation axis passes through the mid-points of the pyrazine carbon—carbon bonds. The pyrazine and pyridine rings are planar, with mean deviations from planarity of 0.007 and 0.001 Å, respectively; the dihedral angle between pyrazine and pyridine rings is 42.2° and between the two pyridine rings is 54.1°.

Experimental. Colorless, parallelepiped crystal, dimensions 0.32 × 0.37 × 0.43 mm. The compound (I) was crystallized from an aqueous manganese(II) perchlorate solution. Nicolet $R3m/V$ diffractometer,



0108-2701/91/092011-02\$03.00

$\omega/2\theta$ scans of 2–15° min⁻¹, $2\theta_{\max} = 45^\circ$, $h = 0$ to 18, $k = -11$ to 0, $l = 0$ to 9, 756 unique measurements, 630 observed [$I > 3\sigma(I)$]. Unit-cell dimensions determined by least-squares fit to settings for 47 reflections ($27 < 2\theta < 45^\circ$). No absorption correction; three standards monitored ($3\bar{3}2$, 522, 114; $\pm 1\%$), 9.0 h of X-ray exposure. Solved by direct methods; full-matrix least-squares refinement on F , $R = 0.0478$, $wR = 0.0694$, $S = 2.49$, $(\Delta/\sigma)_{\max} = 0.01$, 102 variables including positional and anisotropic thermal parameters for the non-H atoms. H atoms were located by difference Fourier techniques and refined isotropically. Function minimized was $\sum w(|F_o| - |F_c|)^2$, where $w = 1/\sigma^2(F_o)$; $\sigma(F_o)$ was estimated from counting statistics. Final difference Fourier peaks ranged from -0.19 to 0.21 e Å⁻³. Computer programs from *SHELXTL* (Sheldrick, 1986), scattering factors (Cromer & Waber, 1974) and real and imaginary anomalous-dispersion corrections (Cromer, 1974). Final atomic coordinates are given in Table 1,* and distances and angles in Table 2; the molecule is shown in Fig. 1.

Related literature. A related compound, 2,3-bis(2-pyridyl)quinoxaline (dpq), has been structurally characterized (Rasmussen, Richter, Yi, Place &

* Lists of structure factors, anisotropic thermal parameters, a summary of crystallographic details and a packing diagram have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 54046 (8 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. Atomic coordinates ($\times 10^4$) and equivalent isotropic thermal parameters ($\text{\AA}^2 \times 10^3$)

U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
N(1)	5827 (1)	5249 (2)	2141 (3)	56 (1)
N(2)	5580 (1)	1718 (2)	985 (3)	50 (1)
C(1)	5405 (2)	6439 (3)	2332 (4)	60 (1)
C(2)	5412 (2)	4024 (3)	2303 (3)	43 (1)
C(3)	5908 (1)	2734 (3)	1989 (3)	43 (1)
C(4)	6694 (2)	2657 (3)	2654 (5)	57 (1)
C(5)	7157 (2)	1482 (4)	2249 (5)	69 (1)
C(6)	6824 (2)	443 (4)	1221 (5)	69 (1)
C(7)	6045 (2)	589 (3)	619 (4)	63 (1)
H(1)	5625 (18)	7374 (32)	2247 (40)	68 (8)
H(2)	6919 (21)	3428 (36)	3396 (48)	77 (10)
H(3)	7667 (24)	1452 (33)	2667 (43)	73 (10)
H(4)	7170 (20)	-334 (39)	874 (48)	82 (10)
H(5)	5691 (23)	-196 (46)	-127 (61)	107 (13)

Table 2. Bond distances (\AA) and angles ($^\circ$)

N(1)—C(1)	1.329 (4)	N(1)—C(2)	1.349 (3)
N(2)—C(3)	1.332 (3)	N(2)—C(7)	1.340 (4)
C(1)—C(1a)	1.353 (6)	C(2)—C(3)	1.485 (3)
C(2)—C(2a)	1.387 (5)	C(3)—C(4)	1.386 (4)
C(4)—C(5)	1.380 (5)	C(5)—C(6)	1.361 (5)
C(6)—C(7)	1.366 (5)	C(1)—H(1)	0.957 (30)
C(4)—H(2)	0.988 (34)	C(5)—H(3)	0.896 (39)
C(6)—H(4)	0.963 (36)	C(7)—H(5)	1.094 (44)
C(1)—N(1)—C(2)	116.9 (2)	C(3)—N(2)—C(7)	117.3 (2)
N(1)—C(1)—H(1)	125 (2)	N(1)—C(1)—C(1a)	122.2 (2)
H(1)—C(1)—C(1a)	113 (2)	N(1)—C(2)—C(3)	114.4 (2)
N(1)—C(2)—C(2a)	120.8 (1)	C(3)—C(2)—C(2a)	124.7 (1)
N(2)—C(3)—C(2)	117.3 (2)	N(2)—C(3)—C(4)	122.8 (2)
C(2)—C(3)—C(4)	119.8 (2)	C(3)—C(4)—C(5)	118.6 (3)
C(3)—C(4)—H(2)	121 (2)	C(5)—C(4)—H(2)	121 (2)
C(4)—C(5)—C(6)	118.8 (3)	C(4)—C(5)—H(3)	118 (2)
C(6)—C(5)—H(3)	123 (2)	C(5)—C(6)—C(7)	119.4 (3)
C(5)—C(6)—H(4)	118 (2)	C(7)—C(6)—H(4)	123 (2)
N(2)—C(7)—C(6)	123.2 (3)	N(2)—C(7)—H(5)	110 (2)
C(6)—C(7)—H(5)	127 (2)		

Brewer, 1990). The most striking difference between these two is the lack of distortion in the title compound. The C(3)—C(2)—C(2a)—C(3a) torsion angle is 5.4° in dpp as opposed to 30.3° for the corresponding angle in dpq. In addition, the pyrazine ring

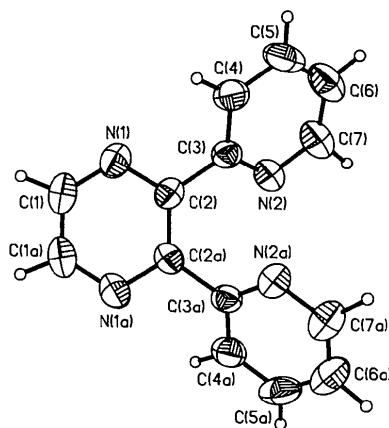


Fig. 1. Molecular structure and numbering scheme, thermal ellipsoids at 50% probability level. H atoms have arbitrary radius.

in dpq was found to deviate significantly from planarity, while the pyrazine ring in dpp has a mean deviation of only 0.007 \AA . As these two molecules should have very similar intramolecular steric interactions, the observed differences are most likely due to intermolecular interactions associated with crystal packing.

Support of this work by the Office of Basic Energy Sciences, Department of Energy is gratefully acknowledged.

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