

trans-2-(2-Phenylethenyl)pyrazineXue-Fang Shi,^{a,b} Hui-Min Liu^b
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Key indicators

Single-crystal X-ray study
T = 293 K
Mean $\sigma(\text{C}-\text{C}) = 0.003 \text{ \AA}$
R factor = 0.045
wR factor = 0.103
Data-to-parameter ratio = 13.5For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

The title compound, $\text{C}_{12}\text{H}_{10}\text{N}_2$, belonging to the orthorhombic system with space group *Pbca*, was prepared by the condensation reaction of benzaldehyde and 2-methylpyrazine in DMF, using KOH as catalyst. The molecule is nearly planar, with a dihedral angle of $7.1(3)^\circ$ between the pyrazine and phenyl planes. In the crystal structure, molecules are connected by $\text{C}-\text{H}\cdots\text{N}$ hydrogen bonds and weak $\pi-\pi$ interactions, resulting in a two-dimensional network.

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Comment

The synthesis of *trans*-2-(2-phenylethenyl)pyrazine (2-PPz), (I), and its derivatives has attracted a great deal of interest (Vansant *et al.*, 1980; Amoroso *et al.*, 1995; Das *et al.*, 1993). Many preparative efforts have focused on methods involving acid catalysis (Taylor & Martin, 1974), but those results were not ideal because of the complicated separation process and the poor yield. Our group has been engaged in improving the synthetic method, using alkali as catalyst instead of acid (Zhang *et al.*, 2000, 2002). We have now synthesized 2-PPz in high yield using KOH as catalyst. The crystal structure of 2-PPz has been determined by single-crystal X-ray diffraction analysis and is reported here. More work on the synthesis of other pyrazine derivatives by the same method is still in progress.

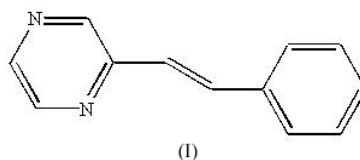


Fig. 1 shows that 2-PPz adopts a *trans* configuration. It is nearly planar, with a dihedral angle of $7.1(3)^\circ$ between the pyrazine and phenyl planes. The $\text{C}=\text{C}$ bond [$1.321(2) \text{ \AA}$] bridging the phenyl and pyrazine rings is of normal length

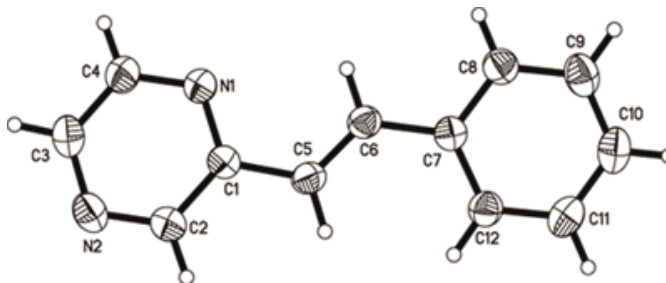


Figure 1

The molecular structure of (I), with displacement ellipsoids drawn at the 30% probability level. H atoms are drawn as small spheres of arbitrary radii.

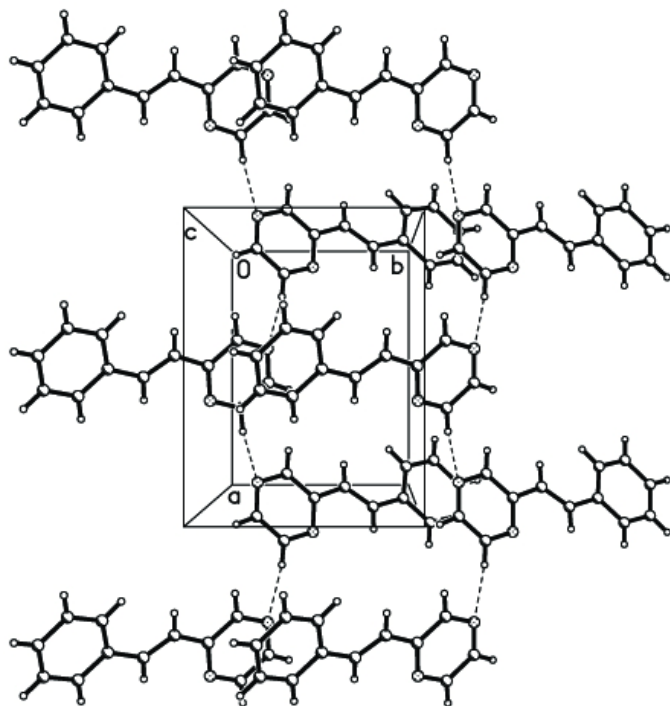


Figure 2
Packing diagram for (I), viewed down the *c* axis. The dashed lines indicate C—H...N hydrogen bonds between neighboring molecules.

(Allen *et al.*, 1987); this value is close to those in compounds with similar configuration, such as *trans*-1,2-bis(4-pyridyl)ethylene (1.329 Å), *trans*-1-(3-pyridyl)-2-(2-pyrazinyl)ethylene (1.331 Å) and *trans*-1,2-bis(2-pyrazinyl)ethylene (1.335 Å) (Vansant *et al.*, 1980).

The packing of the molecules is stabilized by intermolecular C4—H4...N2ⁱ [symmetry code: (i) $x - \frac{1}{2}, -\frac{1}{2} - y, 1 - z$] hydrogen bonds (Table 1), which link the molecules into an infinite chain along the *a* axis. Additionally, weak face-to-face π - π stacking interactions are observed between two anti-parallel molecules, the centroids of the phenyl and pyrazine rings being separated by 4.032 Å. These π - π stacking interactions further connect the 2-PPz molecules into a two-dimensional structure in the *ab* plane, as illustrated in Fig. 2.

Experimental

Under an atmosphere of nitrogen, 1.5 g (14 mmol) benzaldehyde in 2 ml DMF was added dropwise to a mixture of 0.94 g (10 mmol) 2-methylpyrazine and 1.12 g (20 mmol) KOH in 15 ml DMF at 338 K for 2 h. The colorless solution gradually turned yellow. It was then refluxed for another 2 h, cooled slightly and poured into 100 ml cold water. The precipitate was filtered off and recrystallized from methanol/water to give yellow crystals (yield 72%, m.p. 355 K). IR (KBr, ν , cm^{-1}): 3437 (s), 3072 (w), 3030 (w), 1634 (s), 1476 (s), 1399 (s), 1137 (s), 1016 (s), 996 (s), 866 (w), 744 (s), 693 (s). ¹H NMR (CDCl_3 , δ , p.p.m.): 7.12 (*d*, 1H), 7.35 (*m*, 3H), 7.50 (*d*, 2H), 7.74 (*d*, 1H), 8.40 (*s*, 1H), 8.55 (*s*, 1H), 8.65 (*s*, 1H). Single crystals of the title compound were obtained by slow evaporation of an acetone/water solution.

Crystal data

$\text{C}_{12}\text{H}_{10}\text{N}_2$
 $M_r = 182.22$
Orthorhombic, *Pbca*
 $a = 9.794$ (5) Å
 $b = 7.388$ (3) Å
 $c = 26.946$ (12) Å
 $V = 1949.6$ (15) Å³
 $Z = 8$
 $D_x = 1.242$ Mg m⁻³

Mo K α radiation
Cell parameters from 785 reflections
 $\theta = 3.5$ –23.7°
 $\mu = 0.08$ mm⁻¹
 $T = 293$ (2) K
Plate, colorless
 $0.24 \times 0.20 \times 0.08$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
 φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
 $T_{\min} = 0.954$, $T_{\max} = 0.994$
9258 measured reflections

1724 independent reflections
1201 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.040$
 $\theta_{\max} = 25.0^\circ$
 $h = -11 \rightarrow 11$
 $k = -8 \rightarrow 8$
 $l = -22 \rightarrow 32$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.045$
 $wR(F^2) = 0.103$
 $S = 1.09$
1724 reflections
128 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.03P)^2 + 0.5088P]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.13$ e Å⁻³
 $\Delta\rho_{\min} = -0.10$ e Å⁻³

Table 1

Hydrogen-bonding geometry (Å, °).

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
C4—H4...N2 ⁱ	0.93	2.62	3.512 (3)	161

Symmetry code: (i) $x - \frac{1}{2}, -\frac{1}{2} - y, 1 - z$.

H atoms were placed in calculated positions (C—H = 0.93 Å) and allowed to ride on their parent atoms, with U_{iso} values constrained to be $1.2U_{\text{eq}}$ of the parent atom.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1997); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

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