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2,5-Bis[(*E*)-2-phenylethenyl]-3,6-bis(pyridin-2-yl)-pyrazine

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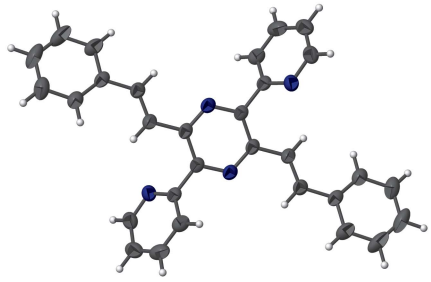
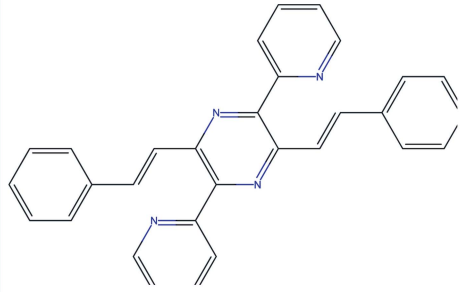
The molecule of the title compound, $C_{30}H_{22}N_4$, exhibits inversion symmetry adopting the shape of a St Andrew's Cross. It shows dihedral angles between adjacent aryl units of around 50° whereas torsion angles of *ca* 10° are found along the arylene vinylene path.

3D view



Chemical scheme



Structure description

The title compound 2,5-(*E*,*E*)-distyryl-3,6-di-(2-pyridyl)pyrazine, $C_{30}H_{22}N_4$, was prepared as a reference chromophore in a project on pyrazine-centered materials, solvatochromic dyes (Schmitt *et al.*, 2008, Wink & Detert, 2013) and liquid crystals (Röder *et al.*, 2019; Schmitt *et al.*, 2011).

The molecule has the shape of a centrosymmetrical St Andrew's cross (Fig. 1). The central pyrazine ring as well as the vinylene groups and the peripheral pyridine and phenyl rings are totally planar. A dihedral angle of 48.07 (6)° at the teraryl axis is nearly identical to those in a related compound with phenyl rings (50.8, 48.6°, Schmitt *et al.*, 2013). Torsion angles along the distyryl axis are −170.21 (15)°, (phenyl-vinyl) and −169.56 (14)° (vinyl-pyrazine). The packing is shown in Fig. 2.

Synthesis and crystallization

The title compound was prepared from 2,5-dimethyl-3,6-di(2-pyridyl)pyrazine (Kolb, 1896) (0.08 g) and benzaldehyde (0.13 g) in 35 ml of DMF by the action of 0.34 g potassium *t*-butylate. The base was added in portions to the stirred and cooled (30 min at 273 K) solution. After 4 h at ambient temperature, the mixture was poured into water, extracted with ethyl acetate and the organic layers were washed, dried (Na_2SO_4) and concentrated. Purification by chromatography on solica gel with toluene/ethyl acetate (20/1) as eluent, R_f = 0.33. Yield: 40 mg, 30%.

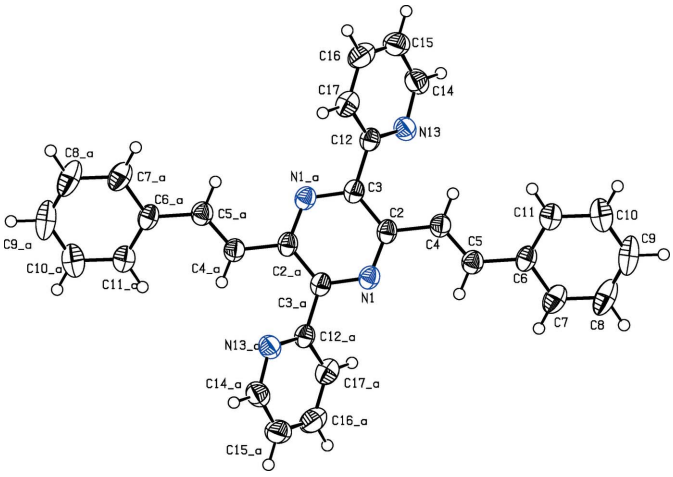


Figure 1
Perspective view of the title compound. Displacement ellipsoids are drawn at the 50% probability level. The second part of the molecule is generated by the symmetry operation $1 - x, 1 - y, 1 - z$.

^{1}H NMR ($CDCl_3$, 400 MHz): 8.83 (*dd*, *J* = 4.9 Hz, *J* = 1.5 Hz, 2 H), 8.23 (*d*, *J* = 7.8 Hz, 2 H), 8.03 (*s* = 2*d*, *J* = 16.1 Hz, 4 H), 7.95 (*dt*, *J* = 7.8 Hz, *J* = 1.9 Hz, 2 H), 7.58 (*d*, 4 H), 7.43 (*ddd*, *J* = 7.8 Hz, *J* = 4.9 Hz, *J* = 1.5 Hz, 2H), 7.36 (*t*, *J* = 7.3 Hz, 4 H), 7.29 (*dt*, *J* = 7.3 Hz, *J* = 1.4 Hz, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz): 157.1, 148.9, 148.3, 145.9, 137.3, 137.0, 135.2, 128.7, 127.6, 125.4, 124.7, 123.6; IR (ATR): 3009, 2988, 2926, 2853, 2688, 1473, 1448, 1276, 1254, 1135, 1086, 1040, 962, 901, 89, 752, 699, 621; MS (APCI): calculated for $C_{30}H_{22}N_4$+H^+): 439.1917, found 439.1908.

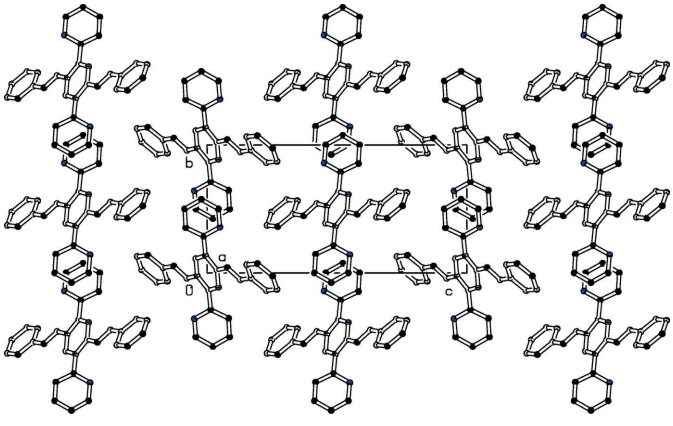


Figure 2
Partial packing diagram of the title compound. View along the *a* axis.

Table 1
Experimental details.

Crystal data	
Chemical formula	$C_{30}H_{22}N_4$
M_r	438.51
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	193
a, *b*, *c* (Å)	7.0953 (8), 8.9310 (8), 18.219 (2)
β (°)	95.490 (9)
V (Å^3)	1149.2 (2)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.08
Crystal size (mm)	0.53 × 0.32 × 0.06
Data collection	
Diffractometer	STOE *IPDS* 2T
Absorption correction	–
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	5878, 2718, 1622
R_{int}	0.029
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.659
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.043, 0.110, 0.99
No. of reflections	2718
No. of parameters	154
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.17, −0.14

Computer programs: *X-AREA* and *X-RED* (Stoe & Cie, 1996), *SIR2004* (Burla *et al.*, 2005), *SHELXL2018* (Sheldrick, 2015) and *PLATON* (Spek, 2020).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1.

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full crystallographic data

IUCrData (2020). **5**, x200372 [https://doi.org/10.1107/S2414314620003727]

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Crystal data

$C_{30}H_{22}N_4$
M_r = 438.51
Monoclinic, $P2_1/c$
a = 7.0953 (8) Å
b = 8.9310 (8) Å
c = 18.219 (2) Å
β = 95.490 (9)°
V = 1149.2 (2) Å^3
Z = 2
$F(000)$ = 460
D_x = 1.267 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3402 reflections
θ = 2.5–28.2°
μ = 0.08 mm^{-1}
T = 193 K
Plate, yellow
0.53 × 0.32 × 0.06 mm

Data collection

STOE IPDS 2T diffractometer
Radiation source: sealed X-ray tube, 12 x 0.4 mm long-fine focus
Detector resolution: 6.67 pixels mm^{-1}
rotation method scans
5878 measured reflections
2718 independent reflections
1622 reflections with $I > 2\sigma(I)$
R_{int} = 0.029
θ_{max} = 27.9°, θ_{min} = 2.5°
h = −9→9
k = −10→11
l = −23→21

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.110
S = 0.99
2718 reflections
154 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0551P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Hydrogen atoms attached to carbons were placed at calculated positions and were refined in the riding-model approximation with C–H = 0.95 Å, and with U_{iso}(H) = 1.2 U_{eq}(C).

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	0.56710 (15)	0.38847 (13)	0.45640 (6)	0.0371 (3)
C2	0.65303 (18)	0.52229 (16)	0.46177 (7)	0.0356 (3)
C3	0.58305 (19)	0.63537 (16)	0.50618 (7)	0.0349 (3)
C4	0.82169 (19)	0.54154 (17)	0.42232 (8)	0.0377 (3)
H4	0.898305	0.627307	0.433494	0.045*
C5	0.8747 (2)	0.44665 (17)	0.37180 (8)	0.0394 (3)
H5	0.796135	0.361702	0.361337	0.047*
C6	1.04162 (19)	0.45956 (17)	0.33065 (8)	0.0385 (4)
C7	1.0601 (2)	0.3624 (2)	0.27172 (8)	0.0524 (4)
H7	0.965446	0.288996	0.259487	0.063*
C8	1.2135 (3)	0.3716 (2)	0.23111 (10)	0.0691 (6)
H8	1.223164	0.305063	0.190953	0.083*
C9	1.3524 (3)	0.4758 (3)	0.24812 (10)	0.0697 (6)
H9	1.458129	0.481619	0.219953	0.084*
C10	1.3377 (2)	0.5724 (2)	0.30648 (10)	0.0585 (5)
H10	1.433770	0.644817	0.318544	0.070*
C11	1.1840 (2)	0.56400 (19)	0.34735 (8)	0.0444 (4)
H11	1.175609	0.630726	0.387515	0.053*
C12	0.66436 (18)	0.78758 (17)	0.51362 (8)	0.0364 (3)
N13	0.69586 (16)	0.85842 (14)	0.45085 (7)	0.0415 (3)
C14	0.7551 (2)	1.00017 (19)	0.45675 (10)	0.0487 (4)
H14	0.774730	1.052537	0.412735	0.058*
C15	0.7892 (2)	1.0746 (2)	0.52227 (11)	0.0545 (5)
H15	0.831478	1.175580	0.523436	0.065*
C16	0.7610 (2)	1.0003 (2)	0.58648 (10)	0.0555 (5)
H16	0.786532	1.048282	0.632899	0.067*
C17	0.6949 (2)	0.85434 (19)	0.58234 (9)	0.0467 (4)
H17	0.671004	0.801209	0.625662	0.056*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0403 (6)	0.0387 (7)	0.0329 (6)	0.0050 (5)	0.0070 (5)	0.0027 (5)
C2	0.0356 (7)	0.0408 (9)	0.0310 (7)	0.0055 (6)	0.0066 (6)	0.0059 (6)
C3	0.0365 (7)	0.0376 (8)	0.0312 (7)	0.0064 (6)	0.0056 (5)	0.0055 (6)
C4	0.0389 (7)	0.0382 (8)	0.0371 (7)	0.0031 (6)	0.0087 (6)	0.0026 (7)
C5	0.0414 (7)	0.0412 (8)	0.0362 (8)	0.0023 (7)	0.0069 (6)	0.0029 (7)
C6	0.0382 (7)	0.0472 (9)	0.0306 (7)	0.0095 (6)	0.0054 (5)	0.0028 (7)
C7	0.0546 (10)	0.0671 (12)	0.0359 (8)	0.0094 (8)	0.0072 (7)	−0.0088 (8)
C8	0.0652 (12)	0.1046 (17)	0.0397 (9)	0.0236 (12)	0.0156 (8)	−0.0111 (10)
C9	0.0503 (10)	0.1129 (18)	0.0494 (10)	0.0206 (12)	0.0227 (8)	0.0132 (12)
C10	0.0414 (8)	0.0791 (13)	0.0562 (10)	0.0031 (9)	0.0107 (7)	0.0166 (10)
C11	0.0429 (8)	0.0512 (10)	0.0400 (8)	0.0060 (7)	0.0079 (6)	0.0034 (7)
C12	0.0312 (7)	0.0392 (8)	0.0391 (8)	0.0059 (6)	0.0057 (6)	0.0000 (7)
N13	0.0395 (7)	0.0396 (7)	0.0462 (7)	−0.0004 (6)	0.0073 (5)	0.0044 (6)

C14	0.0401 (8)	0.0426 (10)	0.0644 (11)	0.0005 (7)	0.0093 (7)	0.0066 (8)
C15	0.0393 (8)	0.0422 (10)	0.0820 (13)	0.0020 (7)	0.0065 (8)	−0.0087 (10)
C16	0.0446 (9)	0.0606 (11)	0.0602 (11)	0.0061 (8)	0.0001 (8)	−0.0226 (9)
C17	0.0437 (8)	0.0532 (10)	0.0433 (9)	0.0070 (7)	0.0049 (6)	−0.0042 (8)

Geometric parameters (Å, º)

N1—C3^{i}	1.3356 (17)	C9—C10	1.381 (3)
N1—C2	1.3410 (18)	C9—H9	0.9500
C2—C3	1.4136 (19)	C10—C11	1.380 (2)
C2—C4	1.4638 (19)	C10—H10	0.9500
C3—C12	1.478 (2)	C11—H11	0.9500
C4—C5	1.332 (2)	C12—N13	1.3442 (18)
C4—H4	0.9500	C12—C17	1.385 (2)
C5—C6	1.4655 (19)	N13—C14	1.335 (2)
C5—H5	0.9500	C14—C15	1.368 (2)
C6—C11	1.387 (2)	C14—H14	0.9500
C6—C7	1.396 (2)	C15—C16	1.376 (3)
C7—C8	1.376 (2)	C15—H15	0.9500
C7—H7	0.9500	C16—C17	1.385 (2)
C8—C9	1.369 (3)	C16—H16	0.9500
C8—H8	0.9500	C17—H17	0.9500
C3^{i}—N1—C2	118.95 (12)	C10—C9—H9	120.2
N1—C2—C3	119.76 (12)	C11—C10—C9	120.21 (17)
N1—C2—C4	117.14 (13)	C11—C10—H10	119.9
C3—C2—C4	123.06 (13)	C9—C10—H10	119.9
N1^{i}—C3—C2	121.29 (13)	C10—C11—C6	120.97 (16)
N1^{i}—C3—C12	115.04 (12)	C10—C11—H11	119.5
C2—C3—C12	123.65 (12)	C6—C11—H11	119.5
C5—C4—C2	124.26 (14)	N13—C12—C17	122.83 (15)
C5—C4—H4	117.9	N13—C12—C3	116.76 (13)
C2—C4—H4	117.9	C17—C12—C3	120.31 (14)
C4—C5—C6	126.81 (14)	C14—N13—C12	117.03 (14)
C4—C5—H5	116.6	N13—C14—C15	124.01 (16)
C6—C5—H5	116.6	N13—C14—H14	118.0
C11—C6—C7	117.79 (14)	C15—C14—H14	118.0
C11—C6—C5	123.22 (13)	C14—C15—C16	118.66 (17)
C7—C6—C5	118.99 (14)	C14—C15—H15	120.7
C8—C7—C6	120.94 (17)	C16—C15—H15	120.7
C8—C7—H7	119.5	C15—C16—C17	118.92 (16)
C6—C7—H7	119.5	C15—C16—H16	120.5
C9—C8—C7	120.52 (17)	C17—C16—H16	120.5
C9—C8—H8	119.7	C16—C17—C12	118.51 (16)
C7—C8—H8	119.7	C16—C17—H17	120.7
C8—C9—C10	119.56 (16)	C12—C17—H17	120.7
C8—C9—H9	120.2		

C3^{i}—N1—C2—C3	−0.4 (2)	C9—C10—C11—C6	−0.2 (2)
C3^{i}—N1—C2—C4	177.52 (12)	C7—C6—C11—C10	0.7 (2)
N1—C2—C3—N1^{i}	0.4 (2)	C5—C6—C11—C10	−179.48 (14)
C4—C2—C3—N1^{i}	−177.38 (12)	N1^{i}—C3—C12—N13	−130.40 (13)
N1—C2—C3—C12	−177.97 (12)	C2—C3—C12—N13	48.11 (17)
C4—C2—C3—C12	4.2 (2)	N1^{i}—C3—C12—C17	46.03 (17)
N1—C2—C4—C5	12.6 (2)	C2—C3—C12—C17	−135.47 (14)
C3—C2—C4—C5	−169.56 (13)	C17—C12—N13—C14	−1.5 (2)
C2—C4—C5—C6	−179.88 (13)	C3—C12—N13—C14	174.83 (12)
C4—C5—C6—C11	9.9 (2)	C12—N13—C14—C15	1.6 (2)
C4—C5—C6—C7	−170.21 (15)	N13—C14—C15—C16	−0.1 (2)
C11—C6—C7—C8	−0.8 (2)	C14—C15—C16—C17	−1.6 (2)
C5—C6—C7—C8	179.34 (15)	C15—C16—C17—C12	1.7 (2)
C6—C7—C8—C9	0.5 (3)	N13—C12—C17—C16	−0.1 (2)
C7—C8—C9—C10	−0.1 (3)	C3—C12—C17—C16	−176.32 (13)
C8—C9—C10—C11	−0.1 (3)		

Symmetry code: (i) −*x*+1, −*y*+1, −*z*+1.