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5,5′-Di-4-pyridyl-2,2′-(*p*-phenylene)di-1,3,4-oxadiazole

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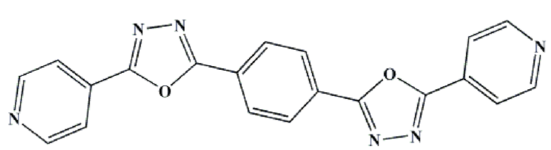
Key indicators: single-crystal X-ray study; T = 183 K; mean σ(C–C) = 0.003 Å; R factor = 0.042; wR factor = 0.112; data-to-parameter ratio = 11.0.

In the crystal structure of the title compound, $C_{20}H_{12}N_6O_2$, the molecules are located on centres of inversion. The complete molecule is almost planar, with a maximum deviation from the mean plane of 0.0657 (1) Å for the O atom. In the crystal, molecules are stacked into columns elongated in the *a* axis direction. The centroid–centroid distances between the aromatic rings of the molecules within the columns are 3.6406 (1) and 3.6287 (2) Å. Molecules are additionally connected *via* weak intermolecular C—H···N hydrogen bonding.

Related literature

For the potential uses of oxadiazoles, see: Bentiss *et al.* (2000); Navidpour *et al.* (2006). For related studies on oxadiazoles, see: Wang *et al.* (2005); Zhang *et al.* (2007). For the synthesis of bis-1,3,4-oxadiazol, see: Al-Talib *et al.* (1990).



Experimental

Crystal data

$C_{20}H_{12}N_6O_2$
M_r = 368.36
Monoclinic, $P2_1/n$
a = 6.2424 (6) Å
b = 7.6969 (7) Å
c = 17.7321 (16) Å
β = 96.635 (2)°
V = 846.27 (14) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 183 K
0.30 × 0.18 × 0.15 mm

Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.971, T_{max} = 0.985
4541 measured reflections
1665 independent reflections
1114 reflections with $I > 2\sigma(I)$
R_{int} = 0.028

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.112
S = 1.01
1665 reflections
151 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.13 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C3—H2···N3^{i}	0.94 (2)	2.52 (2)	3.407 (3)	158.7 (16)

Symmetry code: (i) $-x+\frac{3}{2}, y+\frac{1}{2}, -z+\frac{3}{2}$.

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NC2169).

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supplementary materials

Acta Cryst. (2009). E**65**, o3273 [**doi:10.1107/S1600536809050557**]

5,5'-Di-4-pyridyl-2,2'-(*p*-phenylene)di-1,3,4-oxadiazole

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Comment

The interest in 1, 3, 4-oxadiazole systems originate from their biological activity and their wide application in medicine, industry and coordination chemistry (Bentiss *et al.*, 2000; Navidpour *et al.*, 2006; Wang *et al.*, 2005). Substituted 1, 3, 4-oxadiazole compounds containing pyridyl group displays good coordination activities, but the related study mainly focus on mono-1,3,4 substituted oxadiazole compounds (Wang *et al.*, 2005; Zhang *et al.*, 2007). The synthesis of bis-1,3,4-oxadiazole was reported by Al-Talib *et al.*, 1990, but we have used a modified procedure. In few of the importance of oxadiazole derivatives its crystal structure is reported here.

In the crystal structure of the title compound the molecules are located on centres of inversion and are nearly coplanar. Thus, the asymmetric unit contains half a molecule (Fig. 1). In the crystal structure the molecules are stacked into columns with a centroid-centroid distances of 3.6406 (1) Å] and and 3.6287 (2) Å (Fig. 2). The columns elongate in the direction of the *a* axis and are connected via weak C-H···N hydrogen bonding (Table 1).

Experimental

1, 4-bis[(4-pydiyl)hydrozide]phenylene (1.58 g) was added into 70 ml phosphorous oxychloride ($POCl_3$) and refluxed for about 24 h. After cooling to room temperature, the mixture was poured into 500 ml water. The yellow precipitate was filtered off, washed with water, and dried. Yellow single crystals were obtained by recrystallization of the precipitate from DMF.

Refinement

All H atoms were located in a difference Fourier map and were refined with varying coordinates and varying isotropic displacement parameters.

Figures

Fig. 1. Crystal structure of the title compound showing the atom labeling scheme. Displacement ellipsoids are drawn at the 30% probability level. [symmetry code: A = *x*, *y*, *z*].

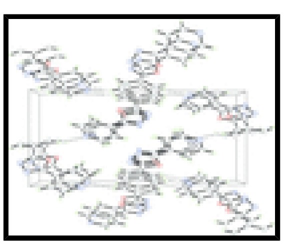

Fig. 2. The molecular packing for the title compound along the *a* axis. The intermolecular C—H···N hydrogen-bonds are shown as dashed lines.

5,5'-Di-4-pyridyl-2,2'-(*p*-phenylene)di-1,3,4-oxadiazole

Crystal data

$C_{20}H_{12}N_6O_2$	$F(000) = 380$
$M_r = 368.36$	$D_x = 1.446$ Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 6.2424$ (6) Å	$\theta = 2.3–26.1°$
$b = 7.6969$ (7) Å	$\mu = 0.10$ mm^{-1}
$c = 17.7321$ (16) Å	$T = 183$ K
$\beta = 96.635$ (2)°	Needle, yellow
$V = 846.27$ (14) Å^3	0.30 × 0.18 × 0.15 mm
$Z = 2$	

Data collection

Bruker SMART APEX CCD diffractometer	1665 independent reflections
Radiation source: fine-focus sealed tube	1114 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.028$
ω scans	$\theta_{max} = 26.1°$, $\theta_{min} = 2.3°$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)	$h = -5\to7$
$T_{min} = 0.971$, $T_{max} = 0.985$	$k = -9\to6$
4541 measured reflections	$l = -21\to20$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.042$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.112$	H atoms treated by a mixture of independent and constrained refinement
$S = 1.01$	$w = 1/[\sigma^2(F_o^2) + (0.0489P)^2 + 0.1652P]$ where $P = (F_o^2 + 2F_c^2)/3$
1665 reflections	$(\Delta/\sigma)_{max} = 0.001$
151 parameters	$\Delta\rho_{max} = 0.18$ e Å^{-3}
0 restraints	$\Delta\rho_{min} = -0.13$ e Å^{-3}

Special details

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

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
O1	1.0105 (2)	0.26943 (17)	0.91503 (7)	0.0455 (4)
N1	1.0141 (3)	0.2372 (2)	1.03852 (9)	0.0481 (5)
N2	0.8290 (3)	0.1534 (2)	1.00208 (9)	0.0490 (5)
C2	1.3123 (3)	0.4031 (2)	0.99232 (11)	0.0393 (5)
C6	0.6794 (3)	0.1193 (3)	0.86751 (11)	0.0427 (5)
C4	1.1139 (3)	0.3024 (2)	0.98550 (10)	0.0406 (5)
C5	0.8350 (3)	0.1759 (2)	0.93029 (11)	0.0419 (5)
C1	1.4231 (3)	0.4324 (3)	1.06365 (12)	0.0445 (5)
C3	1.3910 (3)	0.4712 (3)	0.92850 (11)	0.0436 (5)
N3	0.3677 (3)	0.0203 (3)	0.75019 (11)	0.0710 (6)
C10	0.5034 (4)	0.0236 (3)	0.88153 (14)	0.0559 (6)
C7	0.6983 (4)	0.1636 (3)	0.79320 (13)	0.0578 (6)
C8	0.5402 (4)	0.1127 (4)	0.73749 (14)	0.0672 (7)
C9	0.3534 (4)	−0.0212 (4)	0.82157 (14)	0.0673 (7)
H2	1.316 (3)	0.452 (2)	0.8803 (12)	0.048 (5)*
H1	1.365 (3)	0.390 (2)	1.1064 (12)	0.046 (6)*
H3	0.483 (3)	−0.009 (3)	0.9316 (13)	0.063 (7)*
H6	0.550 (4)	0.142 (3)	0.6864 (15)	0.085 (8)*
H5	0.812 (4)	0.222 (3)	0.7800 (13)	0.069 (8)*
H4	0.234 (4)	−0.079 (3)	0.8314 (14)	0.086 (9)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0404 (8)	0.0544 (9)	0.0408 (8)	−0.0085 (6)	0.0005 (6)	−0.0010 (6)
N1	0.0434 (10)	0.0573 (11)	0.0424 (9)	−0.0076 (8)	−0.0004 (8)	−0.0024 (8)
N2	0.0453 (10)	0.0571 (11)	0.0434 (10)	−0.0091 (8)	0.0001 (8)	−0.0006 (8)
C2	0.0336 (10)	0.0411 (11)	0.0419 (11)	0.0023 (8)	−0.0017 (8)	−0.0022 (8)
C6	0.0395 (11)	0.0451 (12)	0.0425 (11)	−0.0004 (9)	0.0001 (9)	−0.0044 (9)
C4	0.0389 (11)	0.0445 (12)	0.0367 (10)	0.0018 (9)	−0.0027 (9)	−0.0033 (9)
C5	0.0362 (11)	0.0428 (11)	0.0463 (12)	−0.0027 (9)	0.0026 (9)	−0.0004 (9)
C1	0.0423 (12)	0.0521 (13)	0.0383 (11)	−0.0018 (10)	0.0012 (9)	0.0029 (10)
C3	0.0399 (12)	0.0509 (12)	0.0377 (11)	0.0003 (9)	−0.0054 (9)	−0.0013 (9)
N3	0.0657 (14)	0.0925 (16)	0.0512 (12)	−0.0132 (12)	−0.0083 (10)	−0.0080 (11)
C10	0.0573 (14)	0.0641 (15)	0.0452 (13)	−0.0159 (11)	0.0012 (11)	0.0002 (11)
C7	0.0552 (14)	0.0711 (16)	0.0464 (13)	−0.0106 (12)	0.0028 (11)	0.0003 (11)
C8	0.0718 (17)	0.0867 (19)	0.0414 (13)	−0.0059 (14)	−0.0007 (12)	0.0022 (12)
C9	0.0559 (16)	0.088 (2)	0.0559 (16)	−0.0232 (14)	−0.0020 (12)	−0.0079 (13)

Geometric parameters (Å, °)

O1—C4	1.362 (2)	C1—H1	0.94 (2)
O1—C5	1.364 (2)	C3—C1^{i}	1.371 (3)
N1—C4	1.288 (2)	C3—H2	0.94 (2)
N1—N2	1.413 (2)	N3—C9	1.319 (3)
N2—C5	1.290 (2)	N3—C8	1.331 (3)
C2—C3	1.387 (3)	C10—C9	1.377 (3)
C2—C1	1.388 (3)	C10—H3	0.95 (2)
C2—C4	1.454 (3)	C7—C8	1.370 (3)
C6—C10	1.369 (3)	C7—H5	0.89 (2)
C6—C7	1.379 (3)	C8—H6	0.94 (3)
C6—C5	1.457 (3)	C9—H4	0.90 (3)
C1—C3^{i}	1.371 (3)		
C4—O1—C5	102.87 (14)	C2—C1—H1	118.9 (13)
C4—N1—N2	106.44 (15)	C1^{i}—C3—C2	119.80 (18)
C5—N2—N1	105.93 (16)	C1^{i}—C3—H2	120.2 (12)
C3—C2—C1	119.71 (18)	C2—C3—H2	120.0 (12)
C3—C2—C4	120.80 (17)	C9—N3—C8	116.0 (2)
C1—C2—C4	119.48 (18)	C6—C10—C9	118.9 (2)
C10—C6—C7	117.7 (2)	C6—C10—H3	120.6 (14)
C10—C6—C5	120.01 (18)	C9—C10—H3	120.5 (14)
C7—C6—C5	122.2 (2)	C8—C7—C6	119.0 (2)
N1—C4—O1	112.27 (16)	C8—C7—H5	118.8 (15)
N1—C4—C2	128.76 (17)	C6—C7—H5	122.3 (15)
O1—C4—C2	118.96 (16)	N3—C8—C7	124.1 (2)
N2—C5—O1	112.49 (16)	N3—C8—H6	115.6 (16)
N2—C5—C6	128.40 (18)	C7—C8—H6	120.3 (16)
O1—C5—C6	119.09 (17)	N3—C9—C10	124.4 (2)
C3^{i}—C1—C2	120.48 (19)	N3—C9—H4	117.0 (17)
C3^{i}—C1—H1	120.5 (12)	C10—C9—H4	118.5 (17)

Symmetry codes: (i) $-x+3$, $-y+1$, $-z+2$.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H2···N3^{ii}	0.94 (2)	2.52 (2)	3.407 (3)	158.7 (16)

Symmetry codes: (ii) $-x+3/2$, $y+1/2$, $-z+3/2$.

Fig. 1

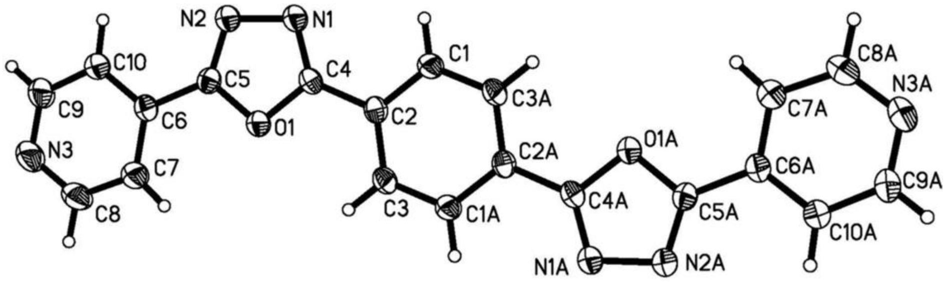
N2
N1
C10
C5
C4
C1
C9
C6
O1
C2
C3A
N3
C7
C2A
O1A
C8
C3
C1A
C4A
C5A
N1A
N2A
C8A
N3A
C7A
C6A
C9A
C10A

Fig. 2