

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

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

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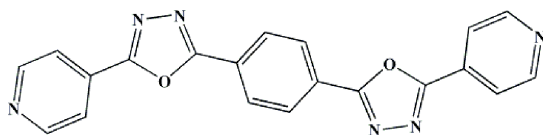
Received 6 November 2009; accepted 24 November 2009

 Key indicators: single-crystal X-ray study; $T = 183$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.042; wR factor = 0.112; data-to-parameter ratio = 11.0.

In the crystal structure of the title compound, $\text{C}_{20}\text{H}_{12}\text{N}_6\text{O}_2$, 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

 $\text{C}_{20}\text{H}_{12}\text{N}_6\text{O}_2$
 $M_r = 368.36$
 Monoclinic, $P2_1/n$
 $a = 6.2424$ (6) Å
 $b = 7.6969$ (7) Å
 $c = 17.7321$ (16) Å

 $\beta = 96.635$ (2)°
 $V = 846.27$ (14) Å³
 $Z = 2$
 Mo $K\alpha$ radiation

 $\mu = 0.10$ mm⁻¹
 $T = 183$ K
 $0.30 \times 0.18 \times 0.15$ 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 $I > 2\sigma(I)$
 $R_{\text{int}} = 0.028$

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
 $\Delta\rho_{\text{max}} = 0.18$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.13$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{C3}-\text{H2}\cdots\text{N3}^i$	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.

This work was supported by the Doctoral Foundation of North University of China.

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

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supporting information

Acta Cryst. (2009). E65, o3273 [doi:10.1107/S1600536809050557]

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

Rui-Sha Zhou and Jiang-Feng Song

S1. 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 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).

S2. Experimental

1, 4-bis[(4-pyridyl)hydrozide]phenylene (1.58 g) was added into 70 ml phosphorous oxychloride (POCl₃) 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.

S3. Refinement

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

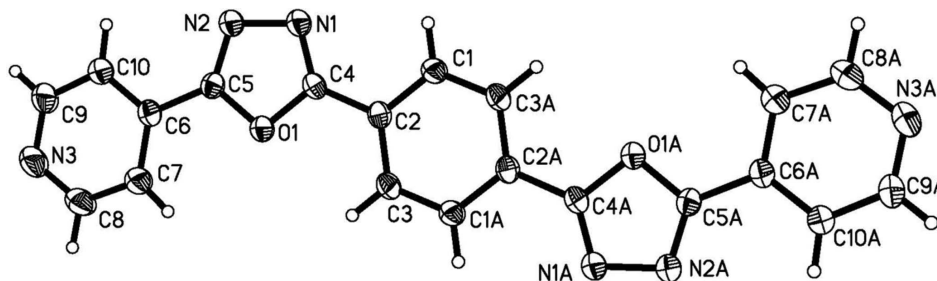
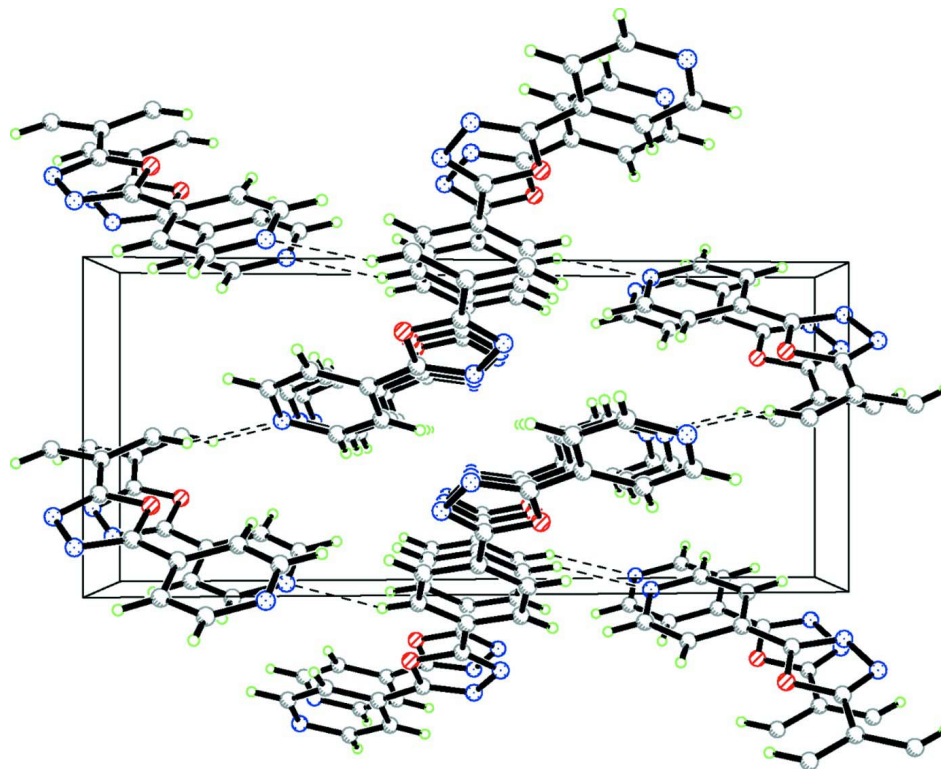


Figure 1

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*].

**Figure 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

$C_{20}H_{12}N_6O_2$

$M_r = 368.36$

Monoclinic, $P2_1/n$

$a = 6.2424$ (6) Å

$b = 7.6969$ (7) Å

$c = 17.7321$ (16) Å

$\beta = 96.635$ (2)°

$V = 846.27$ (14) Å³

$Z = 2$

$F(000) = 380$

$D_x = 1.446$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

$\theta = 2.3$ – 26.1 °

$\mu = 0.10$ mm⁻¹

$T = 183$ K

Needle, yellow

$0.30 \times 0.18 \times 0.15$ mm

Data collection

Bruker SMART APEX CCD

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

ω scans

Absorption correction: multi-scan

(*SADABS*; Sheldrick, 2003)

$T_{\min} = 0.971$, $T_{\max} = 0.985$

4541 measured reflections

1665 independent reflections

1114 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.028$

$\theta_{\max} = 26.1$ °, $\theta_{\min} = 2.3$ °

$h = -5 \rightarrow 7$

$k = -9 \rightarrow 6$

$l = -21 \rightarrow 20$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.042$
 $wR(F^2) = 0.112$
 $S = 1.01$
 1665 reflections
 151 parameters
 0 restraints
 Primary atom site location: structure-invariant
 direct methods

Secondary atom site location: difference Fourier
 map
 Hydrogen site location: inferred from
 neighbouring sites
 H atoms treated by a mixture of independent
 and constrained refinement
 $w = 1/[\sigma^2(F_o^2) + (0.0489P)^2 + 0.1652P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 0.18 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.13 \text{ e } \text{\AA}^{-3}$

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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
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 (\AA^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 code: (i) $-x+3, -y+1, -z+2$.

Hydrogen-bond 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>
C3—H2···N3 ⁱⁱ	0.94 (2)	2.52 (2)	3.407 (3)	158.7 (16)

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