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## Key indicators

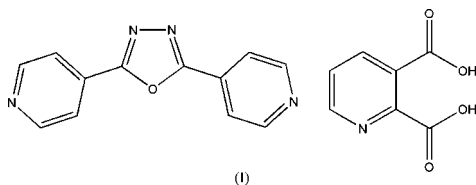
Single-crystal X-ray study  
 $T = 293$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å  
 $R$  factor = 0.043  
 $wR$  factor = 0.128  
Data-to-parameter ratio = 9.8For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.

## 1:1 Cocrystal of 2,5-bis(4-pyridyl)-1,3,4-oxadiazole and pyridine-2,3-dicarboxylic acid

In the title structure,  $\text{C}_7\text{H}_5\text{NO}_4 \cdot \text{C}_{12}\text{H}_8\text{N}_4\text{O}$ ,  $\text{O}-\text{H} \cdots \text{N}$  and  $\text{C}-\text{H} \cdots \text{O}$  hydrogen bonds link the molecules into a two-dimensional supramolecular framework.Received 20 February 2006  
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## Comment

Currently, hydrogen bonding is important in the areas of crystal engineering, supramolecular chemistry, materials science, and biological recognition (Desiraju, 1989; Jeffrey & Saenger, 1991; Holman *et al.*, 2001). Recently, angular dipyr- idyl-donor basic compounds, such as 2,5-bis(4-pyridyl)-1,3,4-oxadiazole (bpo), have been used to produce a series of supramolecules with interesting structures (Du *et al.*, 2006, and references therein; Wang *et al.*, 2005*a,b*, 2006). To identify the properties of co-crystals of aromatic diacids with angular base components and to further understand the role of synthons in crystal engineering, we have prepared and determined the crystal structure of the acid–base co-crystal consisting of bpo and the heterocyclic carboxylic acid, pyridine-2,3-dicarboxylic acid (pdac).



A view of the title structure is shown in Fig. 1. The asymmetric unit consists of one bpo molecule and one molecule of pdac. Bond lengths and angles are unremarkable. The bpo molecule is essentially planar; the dihedral angle between the oxadiazole ring ( $R1$ ) and the  $\text{N}1/\text{C}1-\text{C}5$  ring is  $9.0(1)^\circ$ , while that between  $R1$  and the  $\text{N}4/\text{C}8-\text{C}12$  ring is  $1.8(1)^\circ$ .

$\text{O}-\text{H} \cdots \text{N}$  and  $\text{C}-\text{H} \cdots \text{O}$  hydrogen bonds link the two molecules to form a helical supramolecular tape along the crystallographic  $[010]$  direction, as shown in Fig. 2. These one-dimensional helical chains are further connected by weak  $\text{C}-\text{H} \cdots \text{O}$  interactions to form a two-dimensional corrugated network, as illustrated in Fig. 2. Further analysis of the crystal packing indicates that these two-dimensional undulating layers are interdigitated and adopt an antiparallel stacking mode in the unit cell. Numeric details of the hydrogen bonds are reported in Table 1.

## Experimental

A DMF solution (10 ml) containing 2,5-bis(4-pyridyl)-1,3,4-oxadiazole (22 mg, 0.1 mmol) (Wang *et al.*, 2005*a,b*, 2006) was placed at the

bottom of a straight tube of 18 cm diameter. In the middle of the tube was placed a buffer layer of 1:1 DMF–methanol (10 ml). Pyridine-2,3-dicarboxylic acid (16 mg, 0.1 mmol) in a methanol solution (10 ml) was then added above the buffer layer. After one week, colourless block-shaped crystals suitable for X-ray diffraction were obtained. Analysis found (%): C 58.21, H 3.34, N 17.99%;  $C_{19}H_{13}N_5O_5$  requires (%): C 58.31, H 3.35, N 17.90%.

#### Crystal data

$C_7H_5NO_4 \cdot C_{12}H_8N_4O$   
 $M_r = 391.34$   
 Monoclinic,  $C2/c$   
 $a = 17.576$  (3) Å  
 $b = 10.5434$  (18) Å  
 $c = 20.834$  (4) Å  
 $\beta = 111.674$  (3)°  
 $V = 3587.8$  (11) Å<sup>3</sup>  
 $Z = 8$

$D_x = 1.449$  Mg m<sup>-3</sup>  
 Mo  $K\alpha$  radiation  
 Cell parameters from 3072 reflections  
 $\theta = 2-25^\circ$   
 $\mu = 0.11$  mm<sup>-1</sup>  
 $T = 293$  (2) K  
 Block, colorless  
 $0.30 \times 0.30 \times 0.20$  mm

#### Data collection

Bruker SMART CCD area-detector diffractometer  
 $\varphi$  and  $\omega$  scans  
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)  
 $T_{\min} = 0.968$ ,  $T_{\max} = 0.979$   
 8842 measured reflections

3072 independent reflections  
 2687 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.017$   
 $\theta_{\max} = 25.0^\circ$   
 $h = -19 \rightarrow 20$   
 $k = -12 \rightarrow 12$   
 $l = -23 \rightarrow 24$

#### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.043$   
 $wR(F^2) = 0.129$   
 $S = 1.03$   
 3072 reflections  
 314 parameters  
 All H-atom parameters refined

$w = 1/[\sigma^2(F_o^2) + (0.0803P)^2 + 1.165P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} < 0.001$   
 $\Delta\rho_{\max} = 0.49$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.23$  e Å<sup>-3</sup>

**Table 1**

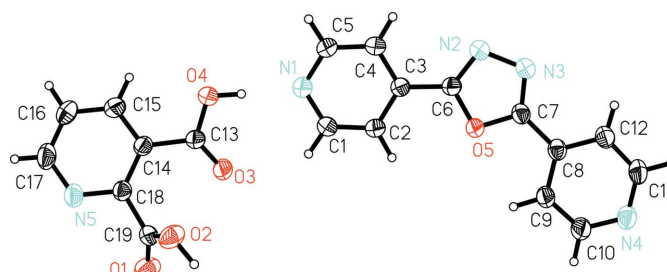
Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
O4–H41 <sup>i</sup> ···N1	0.94 (3)	1.74 (3)	2.679 (2)	177 (2)
O2–H21···N4 <sup>i</sup>	0.97 (3)	1.69 (3)	2.660 (2)	178 (2)
C1–H1···O3	0.94 (3)	2.52 (3)	3.270 (3)	133 (2)
C2–H2···O3 <sup>ii</sup>	0.98 (3)	2.45 (2)	3.127 (3)	125.4 (18)
C9–H9···O5	0.95 (3)	2.51 (3)	2.819 (3)	99.1 (17)

Symmetry codes: (i)  $-x + \frac{1}{2}, y + \frac{1}{2}, -z + \frac{1}{2}$ ; (ii)  $-x, y, -z + \frac{1}{2}$ .

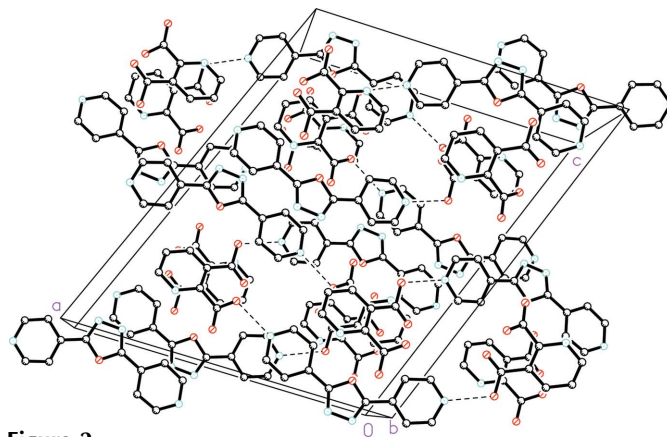
All H atoms were refined independently with isotropic displacement parameters. The C–H and O–H bond lengths lie in the ranges 0.92 (3)–0.99 (2) and 0.94 (2)–0.97 (3) Å, respectively.

Data collection: SMART (Bruker, 2001); cell refinement: SAINT (Bruker, 2001); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Sheldrick, 1999); software used to prepare material for publication: SHELXTL.



**Figure 1**

View of (I), showing displacement ellipsoids drawn at the 30% probability level.



**Figure 2**

Packing diagram (Spek, 2003), showing hydrogen bonds as dashed lines. H atoms have been omitted.

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