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1:1 Cocrystal of 2,5-di-4-pyridyl-1,3,4-oxadiazole and hydroquinone

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.003 Å
R factor = 0.064
wR factor = 0.133
Data-to-parameter ratio = 10.8

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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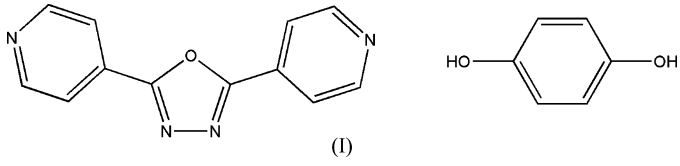
The title complex, 2,5-di-4-pyridyl-1,3,4-oxadiazole–hydroquinone (1/1), $C_{12}H_8N_4O\cdot C_6H_6O_2$, crystallized from a solvent mixture of methanol and water. O—H···N hydrogen bonds link the molecules to give a chain structure.

Comment

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 dipyridyl-donor basic compounds, such as 2,5-bis(4-pyridyl)-1,3,4-oxadiazole (bpo), have been used to produce a series of infinite/discrete coordination polymers/supramolecules with interesting structures and properties (Dong *et al.*, 2003; Du *et al.*, 2005). In our search to identify the properties of cocrystal materials of diols with linear/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 cocrystal consisting of bpo and hydroquinone (Fig. 1).



(I)

A view of the title structure is shown in Fig. 1. The asymmetric unit consists of one bpo and one hydroquinone molecules. In the crystal structure, a one-dimensional chain is formed *via* O—H···N hydrogen bonds (Table 1 and Fig. 2).

Experimental

A mixture of 2,5-bis(4-pyridyl)-1,3,4-oxadiazole (112 mg, 0.5 mmol) (Ren *et al.*, 1995) and hydroquinone (55 mg, 0.5 mmol) was recrystallized from methanol and water in 70% yield (110 mg), from which a light-yellow block-shaped crystal suitable for X-ray diffraction was

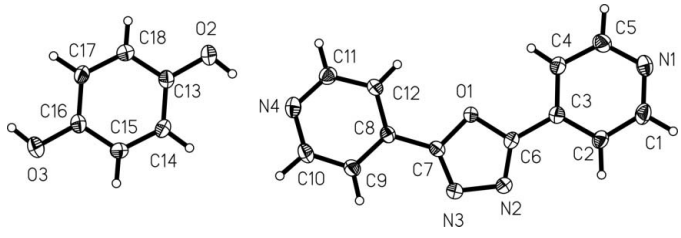


Figure 1
View of (I), showing displacement ellipsoids at the 30% probability level.

selected. Analysis found: C 64.47, H 4.20, N 16.64%; requires: C 64.67, H 4.22, N 16.76%. IR (KBr, cm^{-1}): ν 2450, 1705, 1612, 1569, 1537, 1413, 1276, 1206, 1011, 836, 741, 723.

Crystal data

$C_{12}H_8N_4O{\cdot}C_6H_6O_2$
M_r = 334.33
Orthorhombic, *Pbca*
a = 13.811 (7) Å
b = 5.855 (2) Å
c = 38.550 (15) Å
V = 3117 (2) Å^3
Z = 8
D_x = 1.425 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 250 reflections
θ = 7.5–15°
μ = 0.10 mm^{-1}
T = 298 (2) K
Block, light yellow
0.30 × 0.30 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.971, T_{max} = 0.980
15649 measured reflections
3067 independent reflections
2489 reflections with $I > 2\sigma(I)$
R_{int} = 0.040
θ_{max} = 26.0°
$h = -17 \rightarrow 14$
$k = -7 \rightarrow 7$
$l = -47 \rightarrow 45$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.064
$wR(F^2)$ = 0.133
S = 1.20
3067 reflections
283 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0414P)^2 + 1.24P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0006 (2)

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2A···N4	0.85 (3)	1.94 (3)	2.784 (3)	170 (3)
O3—H3A···N1^{i}	0.89 (4)	1.93 (4)	2.811 (3)	171 (4)

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

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 2001); 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*.

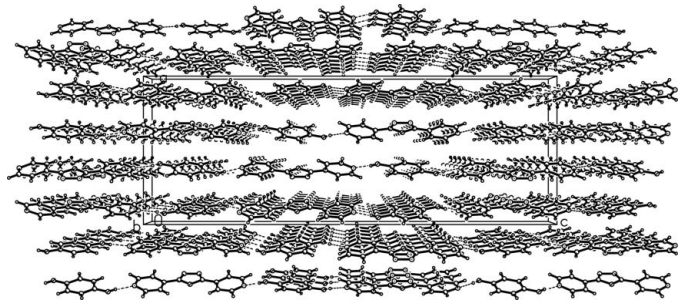


Figure 2
Packing diagram (Spek, 2003), showing hydrogen bonds as dashed lines.

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