Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

1:1 Cocrystal of naphthalene-2,7-diol and 2,5-di-4-pyridyl-1,3,4-oxadiazole

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Received 4 August 2006
Accepted 9 August 2006

The title compound, $C_{10}H_8O_2\cdot C_{12}H_8N_4O$, was crystallized from a methanol and water solvent mixture. In the crystal structure, both types of molecules are linked *via* intermolecular O—H···N hydrogen bonds, forming one-dimensional chains along the [101] direction.

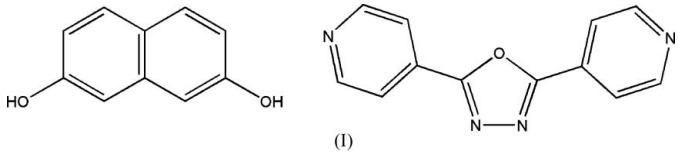
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.004 Å
R factor = 0.051
wR factor = 0.127
Data-to-parameter ratio = 9.6

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

Comment

Crystallization of phenol with pyridine (utilizing O—H···N hydrogen bonding) has been examined in order to build structures with intricate supramolecular architectures, to synthesize host–guest complexes and as a supramolecular template to direct topochemical reactions (Vishweshwar *et al.*, 2003). Recently, a series of supramolecular structures containing 2,5-di-4-pyridyl-1,3,4-oxadiazole (bpo) and some acids, have been successfully constructed (Wang *et al.*, 2005*a*,*b*; Wang, Tang, Qin & Duan, 2006; Wang, Tang, Qin, Duan & Ng, 2006; Wang, Tang & Qin, 2006; Wang, Tang & Wan, 2006). To further expand these results, to identify the properties of cocrystal materials of heterocyclic bases with angular acid components and to further understand the role of synthons in crystal engineering, we have determined the structure of the cocrystal, (I), of bpo and naphthalene-2,7-diol (ndo). We have previously determined the structure of ndo (Wang, Tang & Wan, 2006).



(I)

The molecular structure of (I) is shown in Fig. 1. The asymmetric unit consists of one ndo molecule and one mol-

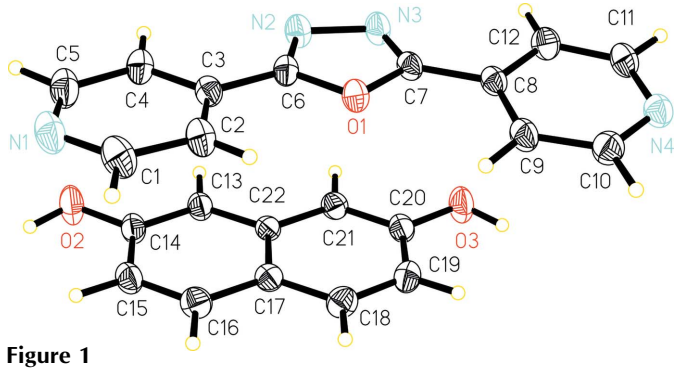


Figure 1
View of the molecular structure of (I), showing displacement ellipsoids at the 30% probability level. H atoms are represented by circles of arbitrary size.

ecule of bpo. In the crystal structure, one-dimensional chains are formed *via* intermolecular O—H···N hydrogen bonds (Table 1 and Fig. 2).

Experimental

A mixture of 2,5-di-4-pyridyl-1,3,4-oxadiazole (112 mg, 0.5 mmol) (Wang *et al.*, 2005*a*) and naphthanene-2,7-diol (80 mg, 0.5 mmol) was recrystallized from methanol (10 ml) and water (2 ml) in 79% yield (152 mg), from which a pale-yellow needle-shaped crystal suitable for *x*-ray diffraction was selected. Analysis found (%): C 68.60, H 4.22, N 14.55; requires (%): C 68.74, H 4.20, N 14.58.

Crystal data

$C_{10}H_8O_2{\cdot}C_{12}H_8N_4O$
M_r = 384.39
Monoclinic, $C2/c$
a = 11.025 (2) Å
b = 8.1452 (16) Å
c = 40.417 (8) Å
β = 91.40 (3)°
V = 3628.5 (12) Å^3
Z = 8
D_x = 1.407 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 298 (2) K
Needle, pale yellow
0.30 × 0.10 × 0.10 mm

Data collection

Bruker SMART APEX CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; (Bruker, 2001)
T_{min} = 0.972, T_{max} = 0.990
8325 measured reflections
3123 independent reflections
1769 reflections with $I > 2\sigma(I)$
R_{int} = 0.056
θ_{max} = 25.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.127
S = 0.99
3123 reflections
327 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0522P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0023 (3)

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···N1^{i}	0.90 (1)	1.86 (1)	2.750 (3)	166 (3)
O3—H3···N4^{ii}	0.91 (3)	1.86 (3)	2.742 (3)	165 (3)

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

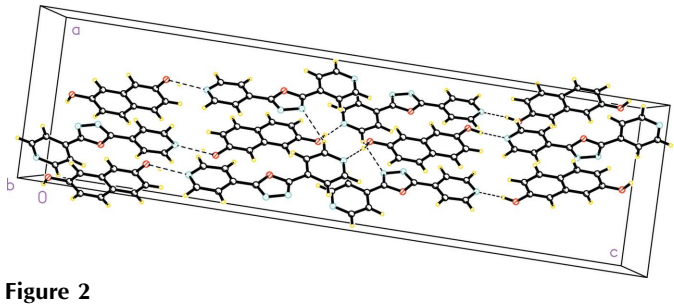


Figure 2
Part of the crystal structure of (I), showing hydrogen bonds as dashed lines.

All H atoms were located in a difference Fourier map and refined independently, with isotropic displacement parameters, giving final C—H distances in the range 0.94 (2)–1.05 (3) Å.

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*.

This work was supported by the Starting Fund of Shandong Institute of Light Industry (to Dr Yong-Tao Wang).

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