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Naphthalene-2,7-diol–imidazole (1/1)

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The asymmetric unit of the title structure, $C_{10}H_8O_2\cdot C_3H_4N_2$, contains two independent naphthalene-2,7-diol molecules and two independent imidazole molecules. In the crystal structure, molecules are linked by intermolecular O—H···N, N—H···O and O—H···O hydrogen bonds, forming one-dimensional chains propagating along [100].

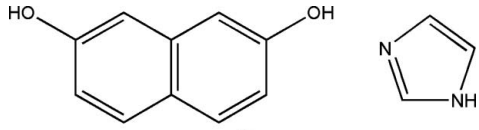
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.003 Å
R factor = 0.055
wR factor = 0.148
Data-to-parameter ratio = 13.4

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

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, the structures of a series of supramolecules which contain angular dipyridyl base compounds and some acids have been determined (Wang *et al.*, 2005*a*,*b*; Wang, Tang, Qin & Duan, 2006; Wang Tang, & Qin, 2006). To further explore the properties of cocrystalline materials of heterocyclic bases with angular acid components and to further understand the role of synthons in crystal engineering, we have prepared a 1:1 cocrystal of naphthalene-2,7-diol (ndo) and imidazole (im).



(I)

A view of the asymmetric unit is shown in Fig. 1; it consists of two independent ndo molecules and two independent molecules of im. In the crystal structure, one-dimensional chains are formed along [100], *via* O—H···O, O—H···N and N—H···O hydrogen bonds (Table 1 and Fig. 2).

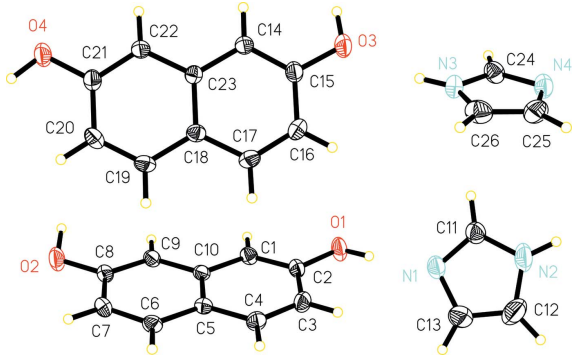


Figure 1
View of the asymmetric unit of (I), showing displacement ellipsoids drawn at the 30% probability level and H atoms as small spheres.

Experimental

To a solution of naphthalene-2,7-diol (80 mg 0.5 mmol) in methanol (5 ml), a solution of imidazole (80 mg 0.5 mmol) in methanol (5 ml) was added. The mixture was filtered. After one week, colourless block-shaped crystals suitable for X-ray diffraction were obtained. Analysis found (%): C 68.29, H 5.34, N 12.19; requires (%): C 68.41, H 5.30, N 12.27.

Crystal data

$C_{10}H_8O_2{\cdot}C_3H_4N_2$
M_r = 228.25
Monoclinic, $P2_1/n$
a = 14.200 (3) Å
b = 7.2927 (18) Å
c = 22.375 (5) Å
β = 101.921 (4)°
V = 2267.1 (9) Å^3
Z = 8
D_x = 1.337 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 298 (2) K
Block, colourless
0.30 × 0.20 × 0.20 mm

Data collection

Bruker SMART APEX CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.973, T_{max} = 0.982
11814 measured reflections
4431 independent reflections
3000 reflections with $I > 2\sigma(I)$
R_{int} = 0.032
θ_{max} = 26.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.148
S = 1.02
4431 reflections
331 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0783P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1	0.90 (2)	1.81 (2)	2.703 (2)	171 (2)
N3—H3···O3	0.85 (3)	2.01 (3)	2.850 (3)	169 (2)
N2—H2···O2^{i}	0.91 (3)	2.15 (3)	2.908 (3)	141 (3)
O2—H2A···O4^{ii}	0.95 (2)	1.78 (2)	2.711 (2)	169 (2)
O3—H3B···O1^{iii}	0.90 (3)	1.89 (3)	2.786 (2)	171 (3)
O4—H4···N4^{iv}	0.94 (3)	1.75 (3)	2.688 (2)	172 (2)

Symmetry codes: (i) $x+1, y, z$; (ii) $-x, -y+1, -z$; (iii) $-x+1, -y+1, -z$; (iv) $x-1, y, z$.

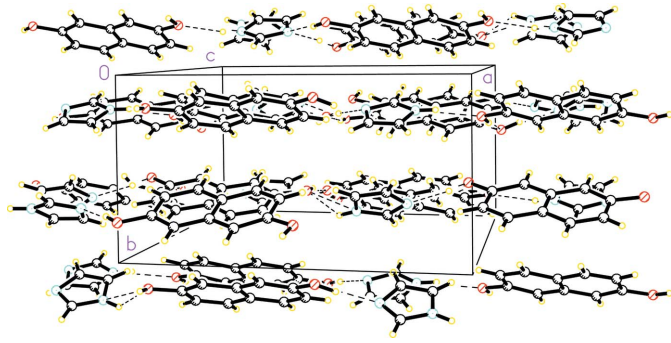


Figure 2
Packing plot, showing hydrogen bonds as dashed lines.

H atoms bonded to N and O atoms were freely refined with isotropic displacement parameters. All C-bound H atoms were placed in geometrically idealized positions and refined in the riding-model appproximation, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C).

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*.

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