Naphthalene-2,7-diol–1,2,4-triazole (2/1)

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In the crystal structure of the title compound, $2C_{10}H_8O_2 \cdot C_2H_3N_3$, intermolecular N—H···O, O—H···N and O—H···O hydrogen bonds connect naphthalene-2,7-diol molecules and 1,2,4-tridazole molecules into a linear ribbon motif.

Comment

Aromatic alcohols are generally not sufficiently acidic to protonate bases; however, naphthalene-2,7-diol represents an exception as it affords some cocrystals with bases, as noted from the reported crystal structures of 10-methylisoalloxazinium bromide hydrate (Langhoff & Fritchie, 1970), cefadroxil heptahydrate (Kemperman *et al.*, 2000) and diaza-18-crown-6 (Watson *et al.*, 1989). In the present study, a 2:1 cocrystal, (I), was obtained when naphthalene-2,7-diol was treated with an equimolar quantity of 1,2,4-triazole. We find it interesting that the title structure is not a 1:1 cocrystal as the reactants were mixed in an equimolar ratio, as was the case for two previously reported crystal structures (Wang & Tang, 2006; Wang, Tang & Wan, 2006).

(I)
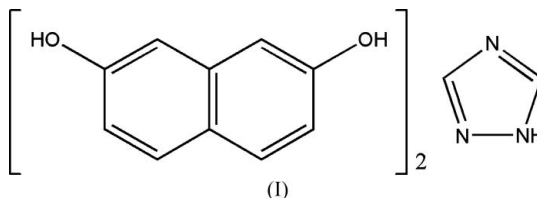
In the crystal structure, a ribbon motif is formed *via* intermolecular N—H···O, O—H···O and O—H···N hydrogen bonds. In detail, the repeat unit of this extended ribbon consists of four O—H···O hydrogen-bonded naphthalene-2,7-diol molecules which are, in turn, O—H···N and N—H···O hydrogen bonded to two 1,2,4-triazole molecules. There are no hydrogen bonds between triazole molecules (Fig. 2 and Table 2).
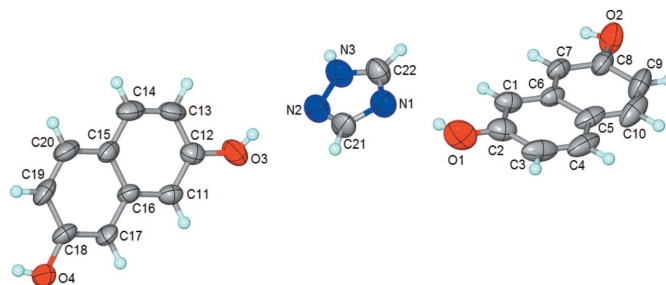

Figure 1
View of the asymmetric unit of (I), shown with displacement ellipsoids at the 50% probability level.

Experimental

Naphthalene-2,7-diol (80 mg, 0.5 mmol) dissolved in methanol (5 ml) was treated with 1,2,4-triazole (35 mg, 0.5 mmol) dissolved in methanol (5 ml). After a few days, colorless bar-shaped crystals separated from the solution. Elemental analysis found: C 62.71, H 4.86, N 18.36%; calculated: C 62.87, H 4.84, N 18.33%.

Crystal data

$2C_{10}H_8O_2 \cdot C_2H_3N_3$
$M_r = 389.40$
Monoclinic, $P2_1/c$
$a = 20.754 (4)$ Å
$b = 5.890 (1)$ Å
$c = 16.273 (4)$ Å
$\beta = 101.682 (6)°$
$V = 1948.0 (7)$ Å^3

$Z = 4$
$D_x = 1.328$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.09$ mm^{-1}
$T = 295 (2)$ K
Bar, colorless
$0.4 \times 0.3 \times 0.3$ mm

Data collection

Bruker SMART 1K area-detector diffractometer
φ and ω scans
Absorption correction: none
8911 measured reflections

3918 independent reflections
1489 reflections with $I > 2\sigma(I)$
$R_{int} = 0.090$
$\theta_{max} = 26.3°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.076$
$wR(F^2) = 0.215$
$S = 0.97$
3918 reflections
267 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0838P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.22$ e Å^{-3}
$\Delta\rho_{min} = -0.19$ e Å^{-3}
Extinction correction: SHELXL97
Extinction coefficient: 0.008 (2)

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
O1—H1$o\cdots$N1	0.85	1.93	2.760 (6)	167
O2—H2$o\cdots$O4^i	0.85	2.02	2.806 (5)	153
O3—H3$o\cdots$N2	0.85	2.12	2.920 (5)	157
O4—H4$o\cdots$O2^{ii}	0.85	1.90	2.743 (4)	172
N3—H3$n\cdots$O3^i	0.85	1.90	2.750 (5)	176

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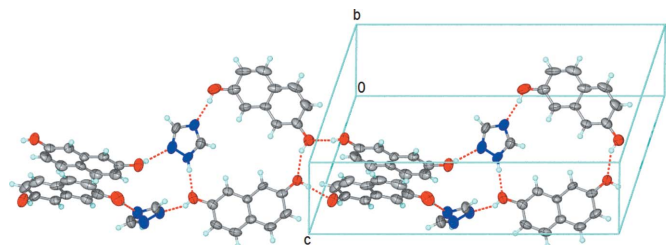

Figure 2
Part of the crystal structure of (I). Hydrogen bonds are shown as dashed lines.

The crystal did not diffract strongly and there are fewer reflections than normal which have $I > 2\sigma(I)$; this may lower the precision of the structure. H atoms were positioned geometrically (C—H = 0.93 Å, N—H = 0.85 Å and O—H = 0.85 Å), and were included in the refinement in the riding-model approximation, with $U_{iso}(H) = 1.2U_{eq}(C,N,O)$.

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: X-SEED (Barbour, 2001); software used to prepare material for publication: SHELXL97.

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