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Pyridin-4-ol–hydroquinone (1/1)

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.047
wR factor = 0.142
Data-to-parameter ratio = 14.0

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

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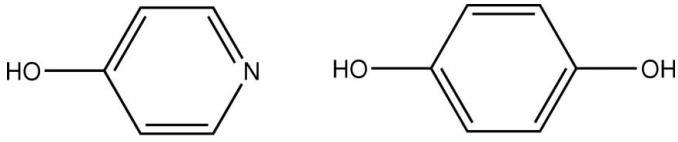
In the title compound, $C_6H_6O_2{\cdot}2C_5H_5NO$, there is one pyridin-4-ol and half a hydroquinone molecule in the asymmetric unit; the hydroquinone molecule lies on an inversion center. The crystal structure is stabilized by intermolecular O—H···N and O—H···O hydrogen bonds, building a corrugated two-dimensional network.

Comment

Quinol, or hydroquinone, shows a great propensity for co-crystallizing with a variety of different compounds. A search of the Cambridge Structural Database (Version 5.25; Allen, 2002) shows that there are 92 co-crystals of quinol with a wide variety of organic compounds (Oswald *et al.*, 2005).

Hydrogen bonding is important in the areas of crystal engineering, supramolecular chemistry, materials science and biological recognition (Wang *et al.*, 2006).

In the title compound, (I), the hydroquinone molecule is arranged around an inversion center (Fig. 1). The bond lengths and angles of the hydroquinone molecule in the complex are similar to values reported in the literature (Moreno-Fuquen *et al.*, 1998).



(I)

The occurrence of O—H···N hydrogen bonds between the pyridin-4(1*H*)-ol molecules leads to the formation of infinite chains, and these chains are interconnected through O—H···O hydrogen bonds involving the hydroquinone molecules, building up a corrugated two-dimensional network (Table 1, Fig. 2). The hydrogen-bonding pattern formed by these O—H···N and O—H···O interactions may be described in graph-set notation as an $R_9^8(42)$ ring (Etter *et al.*, 1990) (Fig. 2).

Experimental

Pyridin-4(1*H*)-ol–hydroquinone crystals were prepared by refluxing a mixture of a solution containing pyridin-4-ol (0.86 g, 9.08 mmol) in ethanol (20 ml) and a solution containing hydroquinone (1 g, 9.08 mmol) in ethanol (20 ml). The reaction mixture was stirred for 30 minutes under reflux. The resulting precipitate was filtered off and crystals of (I) suitable for X-ray analysis were obtained from acetonitrile by slow evaporation (yield 87%, m.p. 411–413 K).

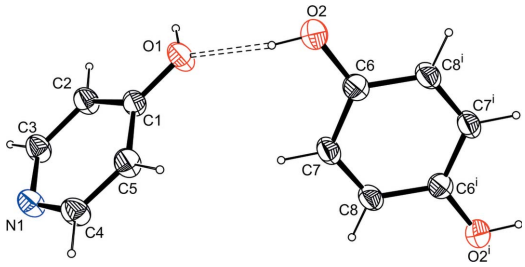


Figure 1
The molecular structure of the title compound showing atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are represented as spheres of arbitrary radii. The hydrogen bond is shown as dashed lines. [Symmetry code: (i) $1-x, 1-y, 1-z$].

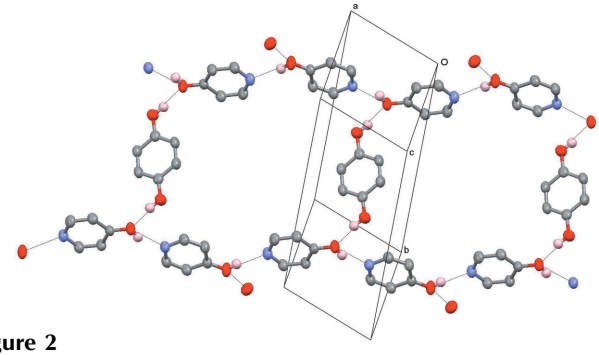


Figure 2
Packing view showing the hydrogen-bonding network. H atoms not involved in hydrogen bonds have been omitted for clarity. Displacement ellipsoids are drawn at the 30% probability level. Hydrogen bonds are shown as dashed lines.

Crystal data

$C_6H_6O_2\cdot 2C_5H_5NO$
$M_r = 300.31$
Monoclinic, $P2_1/c$
$a = 6.2244\ (6)$ Å
$b = 17.3662\ (15)$ Å
$c = 7.1342\ (8)$ Å
$\beta = 109.585\ (8)^\circ$
$V = 726.55\ (12)$ Å^3
$Z = 2$
$D_x = 1.373$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.10$ mm^{-1}
$T = 293\ (2)$ K
Prism, yellow
0.34 × 0.25 × 0.20 mm

Data collection

Stoe IPDS-2 diffractometer
ω scans
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
$T_{min} = 0.941$, $T_{max} = 0.973$
6697 measured reflections
1432 independent reflections
1154 reflections with $I > 2\sigma(I)$
$R_{int} = 0.057$
$\theta_{max} = 26.0^\circ$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.048$
$wR(F^2) = 0.142$
$S = 1.04$
1432 reflections
102 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0828P)^2 + 0.156P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.49$ e Å^{-3}
$\Delta\rho_{min} = -0.43$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···O1	0.82	1.94	2.7339 (19)	161
O1—H1···N1^{ii}	0.82	1.98	2.743 (2)	156

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

H atoms were included in calculated positions and treated using a riding model [O—H= 0.82 Å and C—H(aromatic)= 0.93 Å, with $U_{iso}(H) = 1.2U_{eq}(C)$ and $1.5U_{eq}(O)$].

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996), *ORTEP-3 for Windows* (Farrugia, 1997) and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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