

Quinoxaline–hydroquinone (2/1)

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Key indicators

Single-crystal X-ray study

T = 100 K

Mean $\sigma(\text{C}-\text{C}) = 0.002 \text{ \AA}$

R factor = 0.045

wR factor = 0.112

Data-to-parameter ratio = 12.4

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

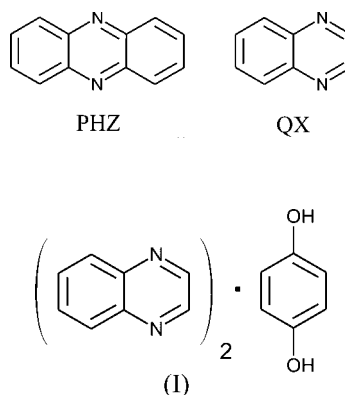
In the 2:1 cocrystal of quinoxaline with hydroquinone, $2\text{C}_8\text{H}_6\text{N}_2 \cdot \text{C}_6\text{H}_4\text{O}_2$, the phenolic molecule is located on an inversion centre. It is connected *via* $\text{O}-\text{H} \cdots \text{N}$ interactions to two molecules of the heterobase, forming discrete hydrogen-bonded assemblies. Quinoxaline molecules are arranged into stacks by $\pi-\pi$ face-to-face interactions whereas the hydroquinone molecules occupy channels formed between these stacks.

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Comment

Quinoxaline (QX) is a heteroaromatic compound which, as a Lewis base, can form metal coordination compounds, and participate in halogen bonding and, as a good acceptor, in hydrogen bonding. Additionally it can be involved as a donor in weak $\text{C}-\text{H} \cdots \text{X}$ interactions and participate in diverse aromatic interactions. Whereas its analogue with an expanded system of condensed rings and higher molecular symmetry, phenazine (PHZ), has been extensively used as a reagent in supramolecular synthesis (Batchelor *et al.*, 2000; Gdaniec *et al.*, 2005; Kutasi *et al.*, 2002; Munakata *et al.*, 1994; Pedireddi *et al.*, 1996; Tomura & Yamashita, 2000; Thalladi, Smolka, Boese & Sustmann, 2000; Thalladi, Smolka, Gehrke, Boese & Sustmann, 2000), much less work has been done with QX. Thalladi, Smolka, Boese & Sustmann (2000) have shown that PHZ forms cocrystals with some biphenols where PHZ molecules, arranged into stacks, form a robust host framework with one-dimensional channels filled by the phenolic molecules.



In the course of our studies on cocrystals of aza-aromatic compounds (Gdaniec *et al.*, 2005) we have prepared cocrystals of quinoxaline with hydroquinone, (I), to check whether molecular organization in these crystals resembles that of the PHZ molecular complex (Thalladi, Smolka, Boese & Sustmann, 2000). X-ray structural analysis revealed a close

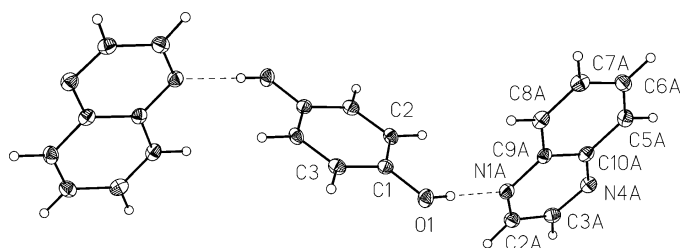


Figure 1
Molecular structure of (I) with displacement ellipsoids shown at the 50% probability level. Hydrogen bonds are shown as dashed lines. Unlabelled atoms are related to labelled atoms by $-x, 1 - y, 2 - z$.

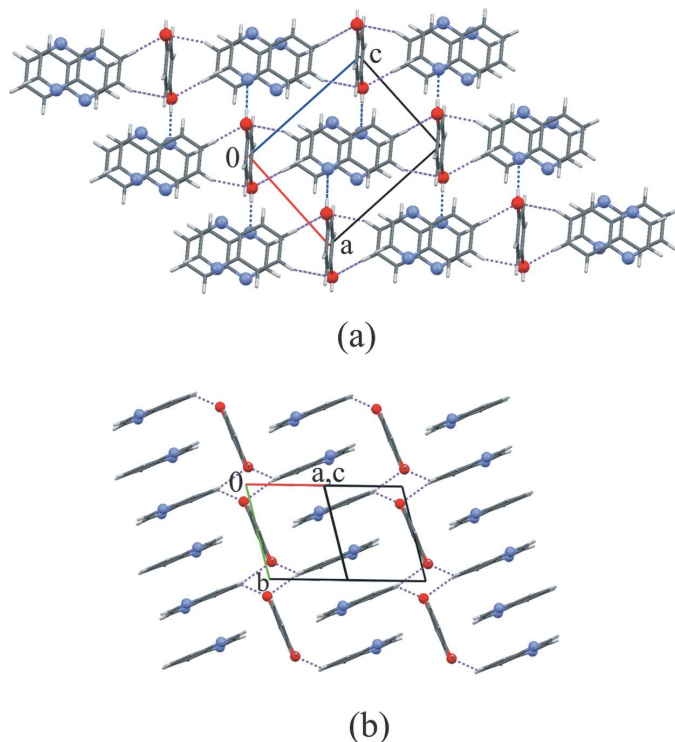


Figure 2
Crystal structure of (I): (a) packing of the molecules viewed down the b axis with the shortest $\text{H}\cdots\text{N}$ and $\text{H}\cdots\text{O}$ contacts shown as dashed lines and (b) arrangement of the molecules within the $(10\bar{1})$ layer.

structural similarity of both cocrystals. Like the PHZ/hydroquinone 2:1 complex, the stoichiometry of the molecular components in (I) is 2:1; the phenolic molecule is located on an inversion centre and is connected *via* $\text{O}-\text{H}\cdots\text{N}$ interactions (Table 1) to two molecules of the heterobase, forming discrete hydrogen-bonded assemblies (Fig. 1). QX molecules are arranged into stacks by offset face-to-face interactions of aromatic systems whereas the hydroquinone molecules occupy channels formed between these stacks (Fig. 2a). The QX and hydroquinone molecules are perpendicular, as shown by the dihedral angle of $89.93(7)^\circ$ between their mean planes. The aromatic interactions, face-to-face between QX molecules and edge-to-face between QX and hydroquinone molecules, as well as $\text{C}-\text{H}\cdots\text{O}$ interactions (Table 1) arrange the molecular components of the cocrystal into layers parallel to the $(10\bar{1})$ plane (Fig. 2b). The strongest intermolecular interactions, $\text{O}-\text{H}\cdots\text{N}$ hydrogen bonds, operate between the

molecules in adjacent $(10\bar{1})$ layers. The crystal structure of (I) shows that, despite differences in molecular structure, PHZ and QX should exhibit close similarity as reagents in supramolecular synthesis.

Experimental

Compound (I) was obtained by slow evaporation of solvent from a methanol solution containing quinoxaline and hydroquinone in a 2:1 molar ratio.

Crystal data

$2\text{C}_8\text{H}_6\text{N}_2\cdot\text{C}_6\text{H}_6\text{O}_2$
 $M_r = 370.40$
Triclinic, $P\bar{1}$
 $a = 7.0724(9) \text{ \AA}$
 $b = 7.2096(10) \text{ \AA}$
 $c = 9.1803(12) \text{ \AA}$
 $\alpha = 72.204(12)^\circ$
 $\beta = 88.516(11)^\circ$
 $\gamma = 85.046(11)^\circ$

$V = 444.03(10) \text{ \AA}^3$
 $Z = 1$
 $D_x = 1.385 \text{ Mg m}^{-3}$
Mo $K\alpha$ radiation
 $\mu = 0.09 \text{ mm}^{-1}$
 $T = 100(2) \text{ K}$
Plate, colourless
 $0.40 \times 0.40 \times 0.15 \text{ mm}$

Data collection

Kuma KM-4-CCD κ -geometry diffractometer
 ω scans
Absorption correction: none
3360 measured reflections

1573 independent reflections
1258 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.043$
 $\theta_{\text{max}} = 25.0^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.045$
 $wR(F^2) = 0.112$
 $S = 1.09$
1573 reflections
127 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0598P)^2 + 0.0086P]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.16 \text{ e \AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.25 \text{ e \AA}^{-3}$

Table 1

Hydrogen-bond geometry ($\text{\AA}, ^\circ$).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{O1}-\text{H1O}\cdots\text{N1A}$	0.85	1.99	2.8425 (18)	179
$\text{C7A}-\text{H7AA}\cdots\text{O1}^{\text{ii}}$	0.95	2.57	3.463 (2)	157
$\text{C6A}-\text{H6AA}\cdots\text{O1}^{\text{iii}}$	0.95	2.58	3.400 (2)	144

Symmetry codes: (ii) $-x, -y + 2, -z + 1$; (iii) $x, y, z - 1$.

All H atoms were located in electron-density difference maps. For the structure refinement they were placed at calculated positions with $\text{C}-\text{H} = 0.95\text{--}0.96 \text{ \AA}$ and $\text{O}-\text{H} = 0.85 \text{ \AA}$ and treated as riding on their parent atoms with $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C}, \text{O})$.

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2004); cell refinement: *CrysAlis CCD*; data reduction: *CrysAlis RED* (Oxford Diffraction, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *Stereochemical Workstation Operation Manual* (Siemens, 1989) and *MERCURY* (Version 1.4; Bruno *et al.*, 2002); software used to prepare material for publication: *SHELXL97*.

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