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1,2,3-Trihydroxybenzene–pyrimidine (1/1)

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Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.003 Å
R factor = 0.052
wR factor = 0.163
Data-to-parameter ratio = 15.4

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

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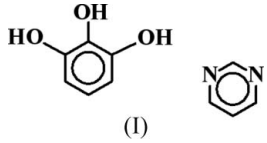
In the title molecular co-crystal, $C_6H_6O_3\cdot C_4H_4N_2$, symmetry-related O—H···N hydrogen bonds with O···N distances of 2.790 (3) and 2.818 (2) Å link molecules of 1,2,3-trihydroxybenzene and pyrimidine to form 18-membered rings which, in turn, are constituents of infinite chains created by O—H···O hydrogen bonds between hydroxy groups in positions 1 and 2 of neighbouring 1,2,3-trihydroxybenzene molecules. The infinite chains are further stacked in stepped columns by offset π-π interactions, and are linked by C—H···π interactions, resulting in a herringbone pattern.

Comment

The strength and directional nature of the hydrogen bond has been a useful tool in crystal engineering as a design element of supramolecular assemblies (Etter, 1991; Lehn, 1995; Desiraju, 1989). In a search for new hydrogen-bonded motifs, we have studied hydrogen-bonded organic co-crystals comprising 'acidic' and 'basic' components. The Cambridge Structural Database contains two previously reported structures with pyrogallol as a component of the adduct. In the first example, pyrogallol–hexametylenetetramine (1/1) (Tremayne & Glidewell, 2000), all hydroxyl groups of the pyrogallol act as hydrogen-bond donors. Molecules are assembled to form two distinct cyclic $R_4^4(18)$ motifs by means of only one type of synthon involving O—H···N hydrogen bonds, with O···N distances 2.90 (1), 2.79 (1) and 2.69 (1) Å. In the second example, pyrogallol–8-hydroxyquinoline (1/1) (Singh *et al.*, 1994), the authors were primarily interested in kinetic studies, and therefore the lack of full crystallographic data precludes any insight into the resulting supramolecular assembly.



(I)

The asymmetric unit of the title compound, (I), comprises two different molecular components, *viz*. 1,2,3-trihydroxybenzene and pyrimidine (Fig. 1). The two molecular building blocks are held together by O1—H1···N1 and O2—H2···N2^{i} [symmetry code:(i) $1-x, 1-y, 1-z$] hydrogen bonds with distances 2.790 (3) and 2.818 (2) Å, respectively, generating an $R_4^4(18)$ tetrameric arrangement with the presence of the same synthon as previously mentioned. The cyclic units are further connected to one another *via* O3—H3···O2^{ii} [symmetry code:(ii) $-x, 1-y, 2-z$] hydrogen bonds [O···O = 2.858 (2) Å, O—H···O = 137.75°] of motif $R_2^2(10)$, forming infinite chains along [001] (Fig. 2). The occurrence of the

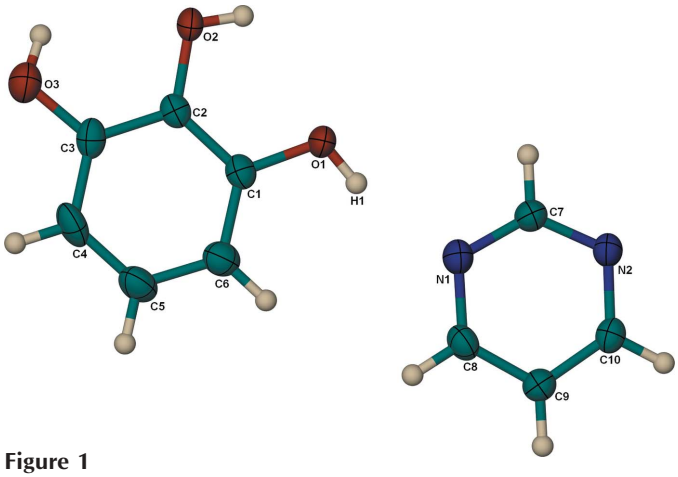


Figure 1
The asymmetric unit of (I), with atom labels and 50% probability displacement ellipsoids for non-H atoms.

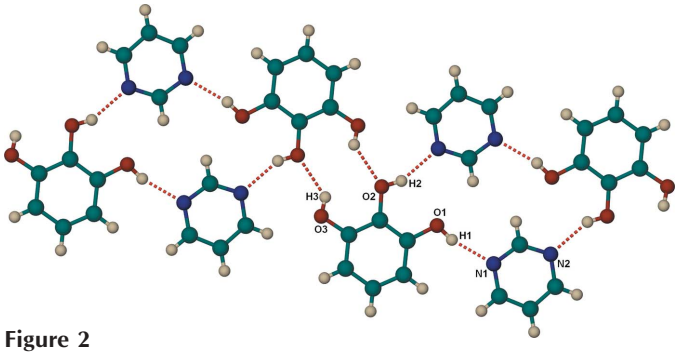


Figure 2
Part of the infinite chain observed in the structure of the title co-crystal. Hydrogen bonds are shown as dashed lines.

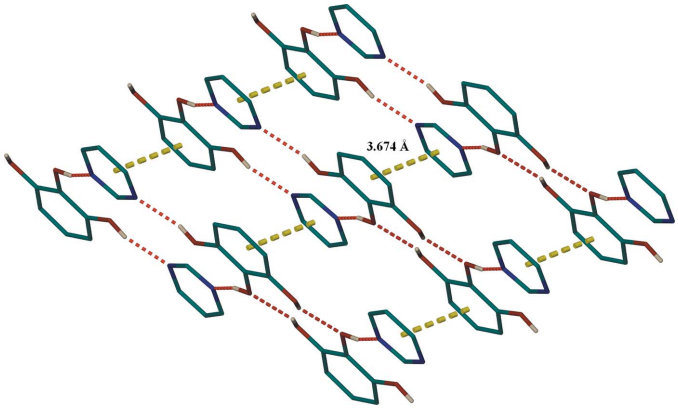


Figure 3
Capped-stick representation showing the π-π stacking geometry of (I). Dashed red lines represent hydrogen bonds. H atoms not involved in hydrogen bonding have been omitted.

second synthon in the structure leads to more efficient packing, since the hydroxyl group in the 2 position of the pyrogallol molecule also acts as a hydrogen-bond acceptor. The poor directionality of O hydrogen-bond acceptors was also noted in the case of 2-aminopyrimidine co-crystals with N—H···O interactions in the range 130–144° (Shan *et al.*, 2002). Benzene and pyrimidine rings from adjacent parallel chains interact by offset π-π interactions (centroid-to-centroid distance 3.674 Å) to form a step-like motif (Fig. 3), which is

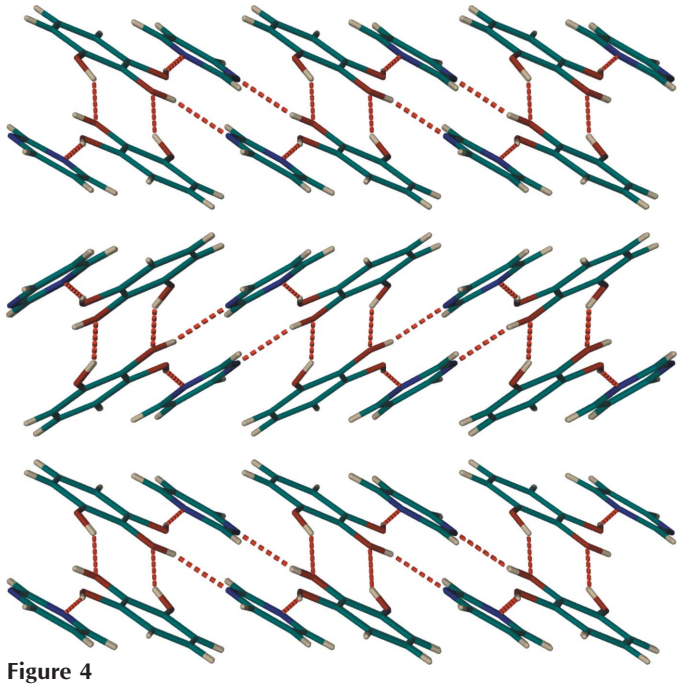


Figure 4
Packing diagram of (I), viewed along [001]. Dashed lines indicate hydrogen bonds.

held together by C—H···π interactions [C8···π (pyrogallol) 3.599 Å, C4···π(pyrimidine) 3.711 Å; measured to the centroid of the ring], resulting in a herringbone packing (Fig. 4).

Experimental

Colourless crystals suitable for single-crystal X-ray diffraction were obtained by slow evaporation of an ethanolic solution of 1,2,3-trihydroxybenzene and pyrimidine (1:1 molar ratio) at room temperature.

Crystal data

$C_6H_6O_3{\cdot}C_4H_4N_2$
M_r = 206.20
Monoclinic, $P2_1/c$
a = 6.5952 (9) Å
b = 13.7481 (19) Å
c = 10.5778 (15) Å
β = 94.051 (3)°
V = 956.7 (2) Å^3
Z = 4
D_x = 1.432 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2112 reflections
θ = 3.0–27.1°
μ = 0.11 mm^{-1}
T = 173 (2) K
Block, colourless
0.30 × 0.25 × 0.20 mm

Data collection

Bruker APEX CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1997)
T_{min} = 0.745, T_{max} = 0.979
5916 measured reflections
2112 independent reflections
1415 reflections with $I > 2\sigma(I)$
R_{int} = 0.030
θ_{max} = 27.1°
$h = -8 \rightarrow 8$
$k = -17 \rightarrow 16$
$l = -8 \rightarrow 13$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.163
S = 1.03
2112 reflections
137 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0584P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 1.02 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1^{i}	0.84	1.98	2.790 (3)	163
O2—H2···N2^{ii}	0.84	2.04	2.818 (2)	155
O3—H3···O2^{iii}	0.84	2.18	2.858 (2)	138

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

H atoms were positioned geometrically (C—H = 0.95 Å, O—H = 0.84 Å) and constrained to ride on their parent atoms; U_{iso}(H) values were set at 1.2 times U_{eq}(C). The highest peak is located 0.31 Å from atom H6.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2002); 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* (Atwood & Barbour, 2003; Barbour, 2001); software used to prepare material for publication: *X-SEED*.

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