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1,2,3-Trihydroxybenzene–1,3,5-triazine (1/1)

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Key indicators

In the title molecular co-crystal, $C_6H_6O_3\cdot C_3H_3N_3$, two hydrogen-bonded $R_4^4(18)$ tetrameric arrangements of molecules involving symmetry-related O—H$\cdots$N hydrogen bonds link molecules of 1,2,3-trihydroxybenzene and 1,3,5-triazine to form an infinite double-chain motif. The one-dimensional array associates with neighbouring strands, *via* C—H$\cdots$O interactions, to form supramolecular sheets that are stacked together by π–π interactions in a three-dimensional assembly.

Comment

Understanding the nature of non-covalent interactions is essential for the development of crystal engineering, in order to facilitate the rational design of supramolecular structures (Desiraju, 1989, 2005; Braga, 2003). As an extension of our studies of supramolecular synthons and crystal packing in molecular co-crystals formed by 'acidic' and 'basic' components, we now report the crystal structure of a (1/1) adduct, (I), of pyrogallol (1,2,3-trihydroxybenzene) and 1,3,5-triazine.

(I)
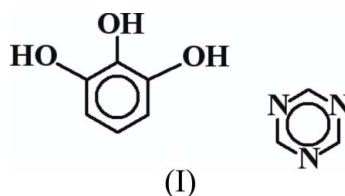
In the crystal structure of a (1/1) complex of pyrogallol and pyrimidine (Dobrzańska, 2005), two distinct synthons were identified, namely a heterosynthon formed *via* O—H$\cdots$N hydrogen bonds and a homosynthon formed *via* weaker poorly directed O—H$\cdots$O hydrogen bonds, coded as $R_4^4(18)$ and $R_2^2(10)$ graph sets, respectively. The crystal structure was stabilized by offset π–π and C—H$\cdots$$\pi$ interactions, resulting in a herringbone packing mode. The same heterosynthon was also found in another co-crystal, of pyrogallol and hexamethylenetetramine, where a three-dimensional supramolecular framework was generated by C—H$\cdots$$\pi$ (arene) interactions (Tremayne & Glidewell, 2000).

The title co-crystal was prepared in order to investigate the effect on the hydrogen-bonding motif of introducing an additional N acceptor site in the heterocyclic ring. The asymmetric unit consists of one molecule of each of pyrogallol and 1,3,5-triazine (Fig. 1). The molecules are held together by hydrogen-bonded O1—H1$\cdots$N1, O2—H2$\cdots$N3[i] and O3—H3$\cdots$N2[ii] interactions (symmetry codes as in Table 1). This facilitates the formation of an infinite double-chain along [010] consisting of $R_4^4(18)$ tetrameric arrangements. The one-dimensional hydrogen-bonded chains of supramolecular
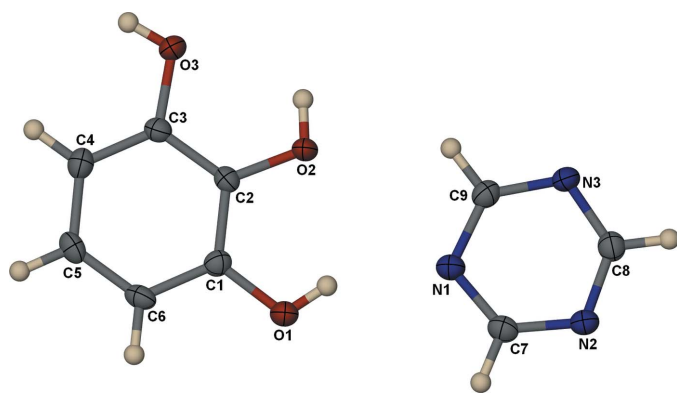
Figure 1
The asymmetric unit of (I), with atom labels and 50% probability displacement ellipsoids.

heterosynthons are further linked to one another *via* C5—H5···O1^{iii} [symmetry code: (iii) $\frac{3}{2} - x, \frac{1}{2} + y, \frac{3}{2} - z$] interactions [C···O = 3.448 (3) Å], to form supramolecular sheets (Fig. 2). Moreover, benzene and triazine rings from adjacent parallel sheets interact *via* offset π–π interactions (centroid···centroid distances 3.418 and 3.621 Å), to form a three-dimensional assembly (Fig. 3).

Only $R_4^4(18)$ heterosynthons formed *via* O—H···N hydrogen bonding are present in the structure of (I), and this motif seems to be favoured in supramolecular structures comprising pyrogallol and compounds containing two or more N acceptor sites.

Experimental

Colourless crystals of (I) suitable for single-crystal X-ray diffraction were obtained by slow evaporation of an ethanolic solution of 1,2,3-trihydroxybenzene and 1,3,5-triazine (1:1 molar ratio) at room temperature.
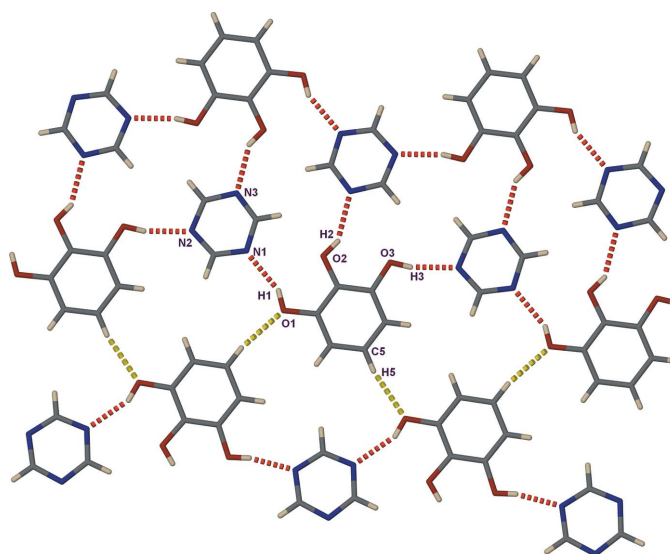

Figure 2
A perspective view of a two-dimensional supramolecular sheet in the structure of (I). Hydrogen bonds are shown as dashed lines (N—H···N indicated in red and C—H···O in yellow).
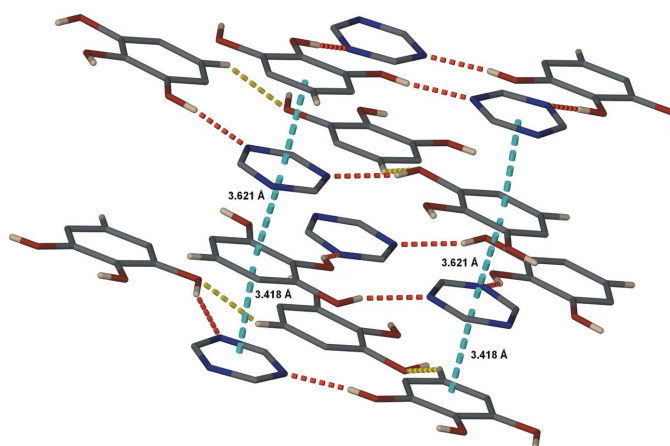

Figure 3
A capped-stick representation, showing the offset π–π interactions in the crystal packing of (I) (dashed blue lines). Dashed red and yellow lines represent N—H···N and C—H···O hydrogen bonds, respectively.

Crystal data

$C_6H_6O_3 \cdot C_3H_3N_3$	$D_x = 1.498$ Mg m^{-3}
$M_r = 207.19$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 2011
$a = 8.7299$ (8) Å	reflections
$b = 10.8999$ (10) Å	$\theta = 2.8–27.1°$
$c = 9.7586$ (8) Å	$\mu = 0.12$ mm^{-1}
$\beta = 98.363$ (2)°	$T = 100$ (2) K
$V = 918.71$ (14) Å^3	Block, colourless
$Z = 4$	$0.27 \times 0.25 \times 0.20$ mm

Data collection

Bruker APEX CCD area-detector diffractometer	2011 independent reflections
	1049 reflections with $I > 2\sigma(I)$
ω scans	$R_{int} = 0.062$
Absorption correction: multi-scan	$\theta_{max} = 27.1°$
(*SADABS*; Sheldrick, 1997)	$h = -8 \rightarrow 11$
$T_{min} = 0.666$, $T_{max} = 0.977$	$k = -13 \rightarrow 11$
5630 measured reflections	$l = -11 \rightarrow 12$

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.050$	$w = 1/[\sigma^2(F_o^2) + (0.0395P)^2]$
$wR(F^2) = 0.107$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.89$	$(\Delta/\sigma)_{max} < 0.001$
2011 reflections	$\Delta\rho_{max} = 0.20$ e Å^{-3}
139 parameters	$\Delta\rho_{min} = -0.20$ e Å^{-3}

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1—H1···N1	0.84	2.08	2.863 (2)	155
O2—H2···N3^i	0.84	2.14	2.892 (2)	149
O3—H3···N2^{ii}	0.84	1.96	2.781 (2)	167

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

H atoms were positioned geometrically, with C—H = 0.95 Å and O—H = 0.84 Å, and were constrained to ride on their parent atoms, with $U_{iso}(H) = 1.2$ times $U_{eq}(C,O)$.

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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References

Atwood, J. L. & Barbour, L. J. (2003). *Cryst. Growth Des.* **3**, 3–8.
Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
Braga, D. (2003). *Chem. Commun.* pp. 2751–2754.
Bruker (2001). *SMART*. Version 5.625. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2002). *SAINT*. Version 6.36a. Bruker AXS Inc., Madison, Wisconsin, USA.
Desiraju, G. R. (1989). *Crystal Engineering. The Design of Organic Solids*. Amsterdam: Elsevier.
Desiraju, G. R. (2005). *Chem. Commun.* pp. 2995–3001.
Dobrzańska, L. (2005). *Acta Cryst.* E**61**, o2981–o2983.
Sheldrick, G. M. (1997). *SHELXS97*, *SHELXL97* and *SADABS* (Version 2.05). University of Göttingen, Germany.
Tremayne, M. & Glidewell, C. (2000). *Chem. Commun.* pp. 2425–2426.