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Trimesic acid dihydrate

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.009 Å
R factor = 0.079
wR factor = 0.156
Data-to-parameter ratio = 6.4

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

The title compound, $C_9H_6O_6 \cdot 2H_2O$, consists of trimesic acid molecules and water molecules of crystallization, linked by O—H···O hydrogen-bond interactions into a three-dimensional network structure.

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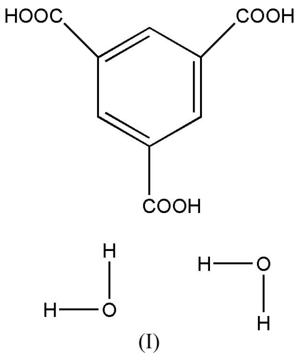
Comment

In the synthesis of crystal structures by design, the assembly of molecular units in predefined arrangements is a key goal (Desiraju, 1995, 1997; Braga *et al.*, 1998). Directional intermolecular interactions are the primary tools in achieving this goal and hydrogen bonding is currently the best among them (Zaworotko, 1997; Braga & Grepioni, 2000). In this paper, we report the structure of trimesic acid dihydrate, (I).



(I)

The title compound consists of trimesic acid molecules and solvent water molecules (Fig. 1). In the crystal structure there are O—H···O and C—H···O intermolecular hydrogen-bond interactions (Table 2), generating a three-dimensional network structure (Fig. 2).

Experimental

The title compound was synthesized by the hydrothermal method from a mixture of trimesic acid (0.3 mmol), 2,2-bipyridine (0.3 mmol), $La_2(SO_4)_3 \cdot 9H_2O$ (0.3 mmol) and water (8.0 ml) in a 15 ml Telfon-lined stainless steel reactor. The solution was heated at 423 K for 4 d. After reaction, the vessel was cooled slowly to room temperature to give colorless crystals. Prismatic crystals were collected, washed with distilled water and dried in air.

Crystal data

$C_9H_6O_6 \cdot 2H_2O$
M_r = 246.17
Orthorhombic, $Pna2_1$
a = 21.000 (4) Å
b = 13.343 (2) Å
c = 3.6863 (6) Å
V = 1032.9 (3) Å^3
Z = 4
D_x = 1.583 Mg m^{-3}

Mo $K\alpha$ radiation
Cell parameters from 5259 reflections
θ = 1.8–25.1°
μ = 0.14 mm^{-1}
T = 298 (2) K
Prism, colorless
0.32 × 0.13 × 0.05 mm

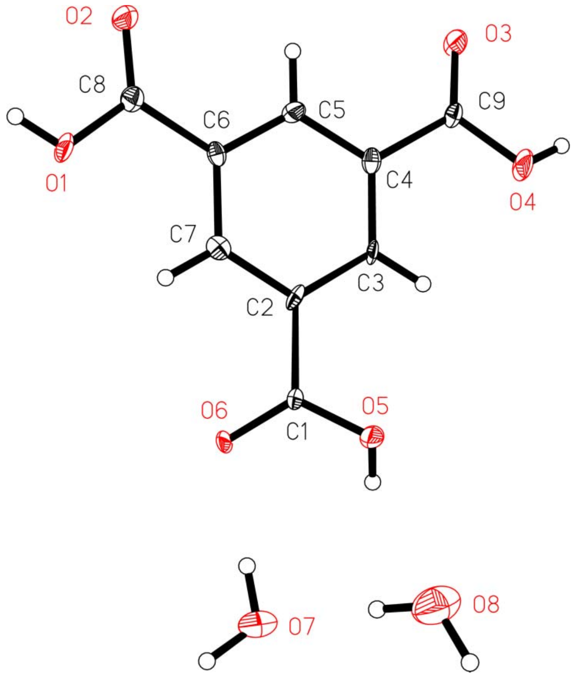


Figure 1
The structure of (I), with the atom numbering, showing displacement ellipsoids at the 50% probability level.

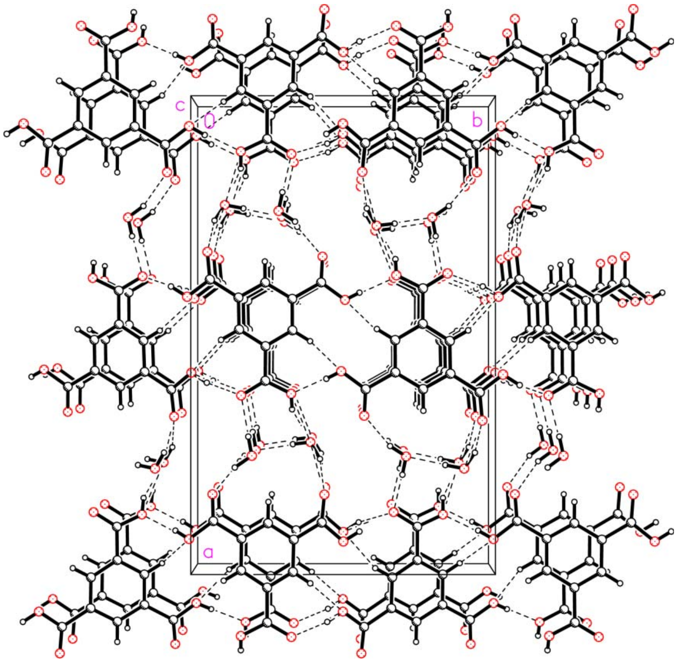


Figure 2
Perspective view of the network structure of (I), showing the intermolecular hydrogen-bond interactions as dashed lines.

Data collection

Bruker SMART APEX area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
$T_{\min} = 0.98$, $T_{\max} = 0.99$
5259 measured reflections
1079 independent reflections
950 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.059$
$\theta_{\max} = 25.1°$
$h = -24 \rightarrow 25$
$k = -15 \rightarrow 14$
$l = -4 \rightarrow 4$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.079$
$wR(F^2) = 0.156$
$S = 1.20$
1079 reflections
169 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0444P)^2 + 2.4467P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.044$
$\Delta\rho_{\max} = 0.30$ e Å^{-3}
$\Delta\rho_{\min} = -0.28$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

O1—C8	1.298 (8)	O4—C9	1.309 (7)
O2—C8	1.211 (7)	O5—C1	1.264 (7)
O3—C9	1.201 (7)	O6—C1	1.234 (7)
O6—C1—O5	122.8 (5)	O3—C9—C4	124.8 (6)
O2—C8—O1	123.4 (6)		

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O8—H8*B*···O2$^{\rm i}$	0.90 (5)	2.01 (7)	2.853 (9)	157 (11)
O7—H7*B*···O6	0.84 (5)	2.00 (7)	2.805 (7)	162 (14)
O7—H7*A*···O3$^{\rm i}$	0.89 (5)	2.13 (6)	2.980 (8)	160 (10)
O8—H8*A*···O7	0.89 (5)	1.91 (5)	2.801 (9)	173 (11)
O1—H1···O6$^{\rm ii}$	0.82	1.81	2.580 (6)	156
O4—H4···O5$^{\rm iii}$	0.82	1.73	2.528 (6)	164
O5—H5*A*···O8$^{\rm iv}$	0.82	2.06	2.845 (9)	160

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

The water H atoms were refined subject to the restraint O—H = 0.82 (5) Å. The other H atoms were positioned geometrically and allowed to ride on their parent atoms at distances of 0.82 (O—H) and 0.93 Å (C—H), with $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}$(parent atom). In the absence of significant anomalous dispersion effects, the Friedel pairs were merged before refinement.

Data collection: *SMART* (Bruker, 2002); 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: *SHELXTL* (Bruker, 2002); software used to prepare material for publication: *SHELXL97*.

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