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2,4,6-Tris(4-pyridylmethylsulfanyl)-1,3,5-triazine monohydrate

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Key indicators

Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.002 Å
R factor = 0.032
wR factor = 0.086
Data-to-parameter ratio = 17.1

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

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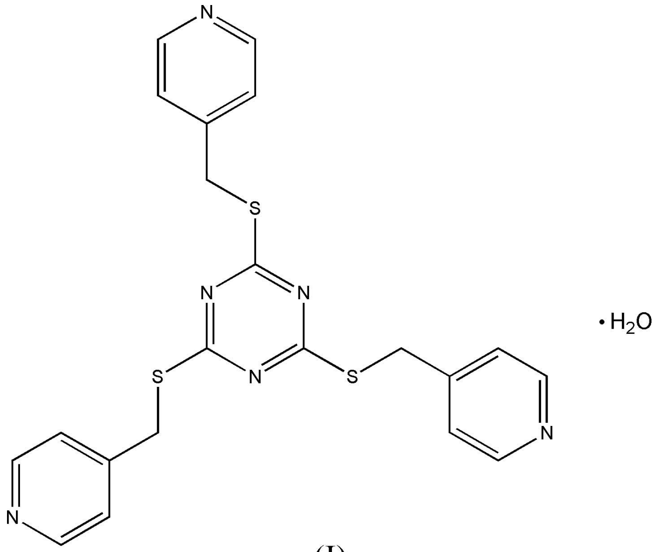
In the crystal structure of the title compound, $C_{21}H_{18}N_6S_3 \cdot H_2O$, the ligands are held together through π–π stacking interactions and O—H···N hydrogen bonds involving the water molecule.

Comment

The ligand 2,4,6-tris(4-pyridylmethylsulfanyl)-1,3,5-triazine (4-TPST) has been used previously in the formation of supramolecular structures containing silver and nickel (Hong *et al.*, 2000*a*). However, the ligand has not previously been crystallized without metal ions in the structure. The asymmetric unit of the title compound, (I), contains one 4-TPST molecule and one water molecule (Fig. 1). The 4-TPST molecule is arranged with two of the pyridine rings bent above the plane of the central triazine ring and the other bent down below the plane. The three $C_{triazine}—S—C_{ethyl}$ angles [102.09 (7)–103.35 (7)°] are all arranged in the same direction around the central triazine ring, as seen in one of the literature examples (Hong *et al.*, 2000*b*) but not in the other (Hong *et al.*, 2000*a*). The central triazine rings are involved in weak π–π interactions, the centroid–centroid distance being 3.9981 (5) Å, in the direction of the *a* axis (Janiak, 2000). There are shorter π–π interactions, the centroid–centroid distance being 3.5617 (4) Å between the pyridine rings of the 4-TPST ligands, linking the ligands together in the [101] direction. There are also numerous hydrogen-bonding interactions between each water molecule and the three surrounding ligand molecules (Desiraju, 2002).



(I)

Experimental

The ligand 2,4,6-tris(4-pyridylmethylsulfanyl-1,3,5-triazine was prepared *via* literature methods (Hong *et al.*, 2000*b*). Single crystals suitable for X-ray analysis were grown by slow evaporation in air of a 1:1 solution of nitromethane and chloroform.

Crystal data

$C_{21}H_{18}N_6S_3{\cdot}H_2O$
$M_r = 468.61$
Triclinic, $P\overline{1}$
$a = 8.4360\ (10)$ Å
$b = 10.8759\ (12)$ Å
$c = 12.1904\ (14)$ Å
$\alpha = 73.9052\ (18)°$
$\beta = 85.9455\ (19)°$
$\gamma = 81.3899\ (19)°$
$V = 1062.0\ (4)$ Å^3
$Z = 2$
$D_x = 1.465$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 5238 reflections
$\theta = 2.3$–$28.0°$
$\mu = 0.38$ mm^{-1}
$T = 150\ (2)$ K
Needle, light yellow
0.55 × 0.11 × 0.09 mm

Data collection

Bruker SMART 1000 CCD diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.89$, $T_{\max} = 0.97$
10553 measured reflections
4892 independent reflections
4257 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.020$
$\theta_{\max} = 28.1°$
$h = -10 \rightarrow 11$
$k = -13 \rightarrow 14$
$l = -16 \rightarrow 16$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.033$
$wR(F^2) = 0.086$
$S = 1.04$
4892 reflections
286 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0371P)^2 + 0.6826P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.42$ e Å^{-3}
$\Delta\rho_{\min} = -0.21$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1A···N4$^{\rm i}$	0.83 (2)	2.16 (2)	2.944 (2)	157 (2)
O1—H1B···N6$^{\rm ii}$	0.84 (2)	2.05 (2)	2.872 (2)	165 (2)

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

All of the H atoms of the 4-TPST molecule were placed in geometrically idealized positions and treated as riding, with C—H = 0.95–0.99 Å and $U_{\rm iso}$(H) = $1.2U_{\rm eq}$(C). The H atoms on the water molecule were located in a difference Fourier map and refined with fixed isotropic displacement parameters of $1.2U_{\rm eq}$(O).

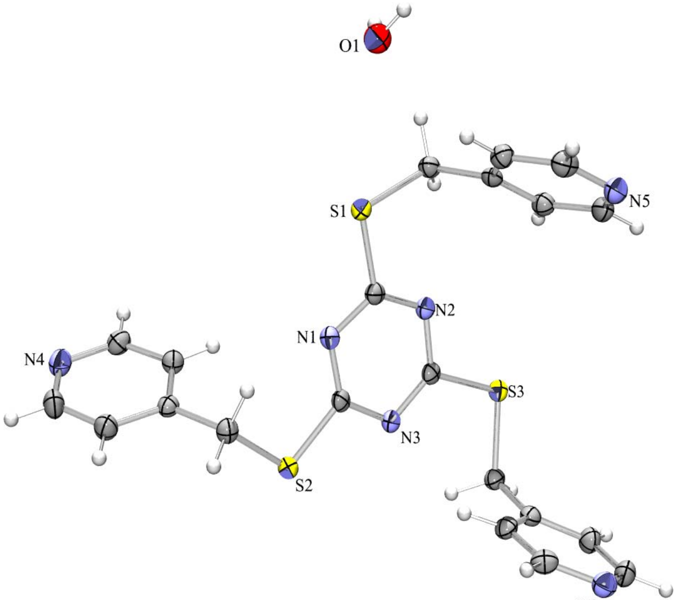


Figure 1
View of the asymmetric unit. Displacement ellipsoids are drawn at the 50% probability level.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT-Plus* (Bruker, 1997); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS86* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *XCIF* (Bruker, 2001).

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