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2,4,6-Tris(pyrimidin-2-ylsulfanyl)-1,3,5-triazine

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.035
wR factor = 0.090
Data-to-parameter ratio = 12.7

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

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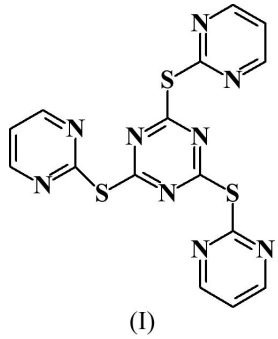
The title compound, $C_{15}H_9N_9S_3$, was synthesized by the reaction of cyanuric chloride with the potassium salt of 2-mercaptopyrimidine. The dihedral angles between the three pyrimidinyl rings and the central triazine plane are 94.1 (4), 105.5 (3) and 126.6 (5)°. The three S atoms are essentially coplanar with the triazine ring, while the orientations of the three pyrimidinyl rings are different, with one ring twisting in the opposite direction to the other two.

Comment

In recent years, large numbers of flexible or rigid multi-thioether ligands with N-containing heterocyclic entities have been synthesized and studied as part of the important field of modern coordination and supramolecular chemistry, owing to their diverse coordinating abilities and structural variety and the specific chemical/physical properties of their metal complexes (Sharma *et al.*, 1999; Hong *et al.*, 2000; Blake *et al.*, 2000; Constable *et al.*, 2002; Bu *et al.*, 2003; Zheng *et al.*, 2003). In addition, S-containing ligands have also been studied with the goal of designing some improved optical sensors for the Ag^I ion (Lerchi *et al.*, 1996). A new trithioether ligand, namely 2,4,6-tris(pyrimidin-2-ylsulfanyl)-1,3,5-triazine, (I), has been synthesized and characterized by X-ray diffraction analysis.



(I)

As shown in Fig. 1, (I) crystallizes with one discrete molecule comprising the asymmetric unit of the unit cell. In the structure, the three pyrimidin-2-ylsulfanyl groups extend out from the central triazine ring, with dihedral angles between the three pyrimidinyl rings (defined as the N6-, N4- and N8-containing rings, respectively) and the central triazine plane of 94.1 (4), 105.5 (3) and 126.6 (5)°, respectively. The three S atoms are essentially coplanar with the triazine ring, while the torsion angles N1—C5—S1—C4, N3—C6—S2—C7 and N1—C11—S3—C12 are all different with values of −21.7 (2), −24.0 (2) and −12.0 (2)°, respectively, reflecting the list of the S—C(*ipso*) bond from the plane of the triazine ring. The orientations of the three pyrimidinyl rings are different, with

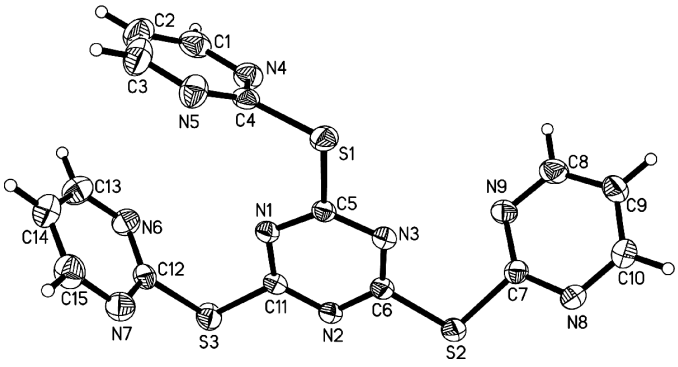


Figure 1
Molecular structure of the title compound (I) with the atom-labeling scheme and ellipsoids drawn at the 30% probability level.

the N6-containing ring twisting in the opposite direction to the N4- and N8-containing rings. This results in the N4- and N6-containing rings lying almost parallel to each other [the dihedral angle between these two rings is 27.3 (2)°].

Experimental

2-Mercaptopyrimidine (1.68 g, 15 mmol) was added to a stirred solution of KOH (0.84 g, 15 mmol) in ethanol (25 ml). In an ice-water bath, the mixture was added dropwise to a solution of cyanuric chloride (0.92 g, 5 mmol) in acetone (20 ml). The mixture was stirred in an ice-water bath for 2 h and for a further 24 h at room temperature. The precipitate which formed was filtered off and washed with water, giving a fine white powder in 63% yield. Colorless single crystals were obtained by recrystallized from chloroform and methanol (m.p. 453–454 K). Analysis calculated for $C_{15}H_9N_9S_3$: C 43.80, H 2.19, N 30.66%; found: C 43.62, H 2.20, N 30.41%; ^{1}H NMR ($CDCl_3$): δ 7.20 (*t*, 3H, CH—C═N), 8.66 (*d*, 6H, C—CH═N); IR (KBr, ν, cm^{-1}): 3078 (*w*), 2967 (*w*), 1802 (*w*), 1616 (*w*), 1553 (*s*), 1474 (*s*), 1430 (*m*), 1384 (*s*), 1268 (*s*), 1205 (*m*), 1165 (*s*), 988 (*m*), 840 (*s*), 807 (*s*), 777 (*s*), 746 (*s*), 628 (*s*), 560 (*m*), 515 (*m*), 472 (*w*).

Crystal data

$C_{15}H_9N_9S_3$
M_r = 411.49
Monoclinic, $P2_1/n$
a = 9.020 (1) Å
b = 18.233 (3) Å
c = 11.219 (2) Å
β = 107.908 (2)°
V = 1755.7 (5) Å^3
Z = 4
D_x = 1.557 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1536 reflections
θ = 2.6–22.5°
μ = 0.44 mm^{-1}
T = 293 (2) K
Plate, colorless
0.42 × 0.20 × 0.04 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1997)
T_{min} = 0.845, T_{max} = 0.978
9470 measured reflections
3110 independent reflections
2177 reflections with $I > 2\sigma(I)$
R_{int} = 0.033
θ_{max} = 25.0°
$h = -10 \rightarrow 9$
$k = -21 \rightarrow 21$
$l = -7 \rightarrow 13$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.090
S = 1.08
3110 reflections
244 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0309P)^2 + 0.2133P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

H atoms were positioned geometrically and refined using a riding model, with C—H distances of 0.93 Å and with $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); 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, 1997); software used to prepare material for publication: *SHELXTL*.

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References

Blake, A. J., Champness, N. R., Howdle, S. M. & Webb, P. B. (2000). *Inorg. Chem.* **39**, 1035–1042.
Bruker (1997). *SMART*, *SAINT* and *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bu, X. H., Xie, Y. B., Li, J. R. & Zhang, R. H. (2003). *Inorg. Chem.* **42**, 7422–7430.
Constable, E. C., Housecroft, C. E., Kariuki, B. M., Kelly, N. & Smith, C. B. (2002). *Inorg. Chem. Commun.* **5**, 199–202.
Hong, M. C., Zhao, Y. J., Su, W. P., Cao R., Fujita, M., Zhou, Z. Y. & Chan, A. S. C. (2000). *J. Am. Chem. Soc.* **122**, 4819–4820.
Lerchi, M., Orsini, F., Cimerman, Z. & Pretsch, E. (1996). *Anal. Chem.* **68**, 3210–3214.
Sharma, C. V. K., Broker, G. A., Huddleston, J. G., Baldwin, J. W., Metzger, R. M. & Rogers, R. D. (1999). *J. Am. Chem. Soc.* **121**, 1137–1144.
Sheldrick, G. M. (1997). *SHELXS97*, *SHELXL97* and *SADABS*. University of Göttingen, Germany.
Zheng, Y., Du, M., Li, J. R., Zhang, R. H. & Bu, X. H. (2003). *Dalton Trans.* pp. 1509–1514.