N3—S2—O4	108.3 (1)	C15—S14—O29	106.9 (1)
N3—S2—O5	105.9 (1)	S14—C15—C16	119.1 (2)
N3—S2—C11	106.8 (1)	S14—C15—C20	119.8 (2)
O4—S2—O5	119.9 (1)	C16—C15—C20	120.9 (2)
O4—S2—C11	108.0 (1)	C15—C16—C17	117.3 (2)
O5—S2—C11	107.2 (1)	C16—C17—C18	124.7 (2)
S2—N3—C6	119.6 (2)	C16—C17—F22	116.9 (2)
N3—C6—C13	110.2 (2)	C18—C17—F22	118.4 (2)
C8—C7—C12	119.8 (2)	C17—C18—C19	115.2 (2)
C11—C8—C7	120.1 (2)	C17—C18—O23	130.2 (2)
C11—C8—C9	119.3 (2)	C19—C18—O23	114.6 (2)
C7—C8—C9	120.6 (2)	C18—C19—C20	122.7 (2)
C8—C9—C10	119.9 (2)	C18—C19—F21	116.6 (2)
C9—C10—C11	120.7 (2)	C20—C19—F21	120.6 (2)
S2—C11—C10	119.5 (2)	C15—C20—C19	119.1 (2)
S2—C11—C12	121.1 (2)	C18—O23—C24	121.5 (2)
C10—C11—C12	119.2 (2)	O23—C24—C25	113.1 (2)
C7—C12—C11	119.7 (2)	C24—C25—O26	127.1 (2)
C6—C13—S14	109.6 (2)	C24—C25—O27	109.6 (2)
C13—S14—C15	97.7 (1)	O26—C25—O27	123.3 (2)
C13—S14—O29	105.4 (1)	C25—O27—C28	117.0 (2)

The *MAXUS* software package (Mackay *et al.*, 1997) was used throughout the analysis.

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termolecular O—H···N hydrogen bonds link the molecules into infinite chains.

Comment

Derivatives of benzothiazole belong to a series of compounds which have especially remarkable biological properties (Varkonda *et al.*, 1985). We report here on the crystal structure of 1-(1,3-benzothiazol-2-yl)-3,3,3-trichloro-2-propanol, (I).

(I)

The mean value of 1.377 (4) Å for the six C—C bonds in the benzene ring is significantly short of the value of 1.397 Å expected from neutron diffraction (Bacon *et al.*, 1964). The two C—S distances [1.713 (3) and 1.733 (3) Å] in the thiazole ring have values intermediate between those reported for C_{sp^3}—S single [1.81 Å] and double [1.61 Å] bonds (Khan *et al.*, 1988). The bond distances C4—N1 [1.272 (3) Å] and N1—C5 [1.394 (3) Å] are in agreement with those found in related compounds (Bhatia *et al.*, 1991; Teo *et al.*, 1995). The benzothiazole nucleus adopts an almost planar conformation, with a dihedral angle between the individual planes of the benzene and thiazole rings of 1.20 (8)°. The crystal packing is dominated by O—H···N hydrogen bonds [O1···N1^i 2.807 (3), H1···N1^i 1.64 (4) Å, O—H···N^i 166 (2)°; symmetry code: (i) x, $-y$, $\frac{1}{2} + z$], which link the molecules into infinite chains in the **b** direction.

1-(1,3-Benzothiazol-2-yl)-3,3,3-trichloro-2-propanol

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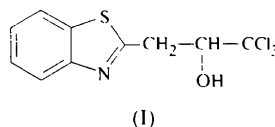
Abstract

In the title compound, $C_{10}H_8Cl_3NOS$, the two planar benzene and thiazole rings are nearly coplanar. The dihedral angle between them is 1.20 (8)°. Strong in-
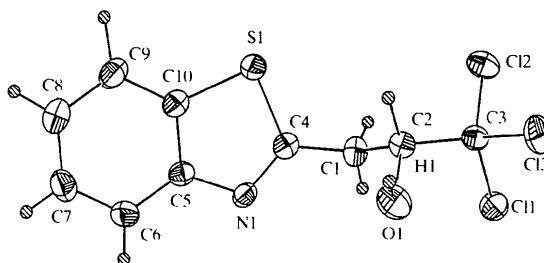
Fig. 1. *ORTEP*II (Johnson, 1976) plot of the title molecule, showing the labelling of the non-H atoms. Displacement ellipsoids are shown at 50% probability levels; H atoms are drawn as small circles of arbitrary radii.

Experimental

Full details of the synthetic procedure have been published by Ettel *et al.* (1950). Single crystals were prepared by crystallization from ethanol.

Crystal data

$C_{10}H_8Cl_3NOS$
$M_r = 296.58$
Monoclinic
$C2/c$
$a = 21.595\,(13)$ Å
$b = 12.323\,(7)$ Å
$c = 9.266\,(6)$ Å
$\beta = 98.90\,(5)°$
$V = 2436\,(3)$ Å^3
$Z = 8$
$D_x = 1.617$ Mg m^{-3}
$D_m = 1.63\,(1)$ Mg m^{-3}
D_m measured by flotation in bromoform/hexane

Mo $K\alpha$ radiation
$\lambda = 0.71069$ Å
Cell parameters from 15 reflections
$\theta = 11.8–26.4°$
$\mu = 0.899$ mm^{-1}
$T = 293\,(2)$ K
Block
$0.35 \times 0.25 \times 0.20$ mm
Colourless

Data collection

Syntex $P2_1$ diffractometer
$\theta/2\theta$ scans
Absorption correction: none
2822 measured reflections
2822 independent reflections
1352 reflections with
   $I > 2\sigma(I)$

$\theta_{max} = 27.60°$
$h = 0 \rightarrow 28$
$k = 0 \rightarrow 16$
$l = -12 \rightarrow 11$
2 standard reflections
   frequency: 100 min
   intensity decay: none

Refinement

Refinement on F^2
$R(F) = 0.039$
$wR(F^2) = 0.070$
$S = 1.149$
2822 reflections
178 parameters
H atoms refined isotropically
$w = 1/[\sigma^2(F_o^2) + (0.0332P)^2]$
   where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.024$
$\Delta\rho_{max} = 0.215$ e Å^{-3}
$\Delta\rho_{min} = -0.221$ e Å^{-3}
Extinction correction: none
Scattering factors from
   International Tables for
   Crystallography (Vol. C)

Table 1. *Selected geometric parameters (Å, °)*

S1—C10	1.713 (3)	C5—C6	1.373 (4)
S1—C4	1.733 (3)	C5—C10	1.400 (4)
O1—C2	1.374 (3)	C6—C7	1.355 (4)
N1—C4	1.272 (3)	C7—C8	1.374 (4)
N1—C5	1.394 (3)	C8—C9	1.383 (4)
C1—C4	1.493 (4)	C9—C10	1.375 (4)
C10—S1—C4	89.40 (14)	N1—C4—S1	116.2 (2)
C4—N1—C5	110.7 (2)	N1—C5—C10	114.4 (2)
O1—C2—C1	109.8 (2)	C5—C10—S1	109.2 (2)
O1—C2—C3	110.8 (2)		

Non-H atoms were refined anisotropically, H atoms were located from a difference Fourier map and all parameters were refined isotropically.

Data collection: Syntex $P2_1$ software. Cell refinement: Syntex $P2_1$ software. Data reduction: *XP21* (Pavelčík, 1987). Program(s) used to solve structure: *SHELXS86* (Sheldrick, 1990). Program(s) used to refine structure: *SHELXL93* (Sheldrick, 1993). Molecular graphics: *ORTEP*II (Johnson, 1976). Software used to prepare material for publication: *SHELXL93*.

Supplementary data for this paper are available from the IUCr electronic archives (Reference: KA1264). Services for accessing these data are described at the back of the journal.

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

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Abstract

Molecules of the title compound, $C_{18}H_{12}N_6$, were significantly distorted from planarity, with the three least-squares mean planes of the pyridine rings twisted from the plane of the central triazine ring by 15.7 (1), 33.8 (1) and 19.8 (1)°.

Comment

There is much current interest in the use of triazine ligands such as 2,4,6-tris(2-pyridyl)-1,3,5-triazine (L^1, TPTZ) for the extraction and separation of metal ions (Byers *et al.*, 1994, 1996; Chan *et al.*, 1996). TPTZ and its substituted derivatives such as 2,4,6-tris(4-*tert*-butyl-2-pyridyl)-1,3,5-triazine (L^2) are used in the nuclear industry as solvent-extraction reagents since they are able to separate trivalent actinides (An^{III}) and lanthanides (Ln^{III}) from nitric acid media. The ligands have been found to form metal complexes in which they act as approximately planar tridentate ligands (Chan *et*