organic papers

1,3,5-Trichloro-1λ^6,2,4,6-thiatriazin-1-one

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In the title compound, $C_2Cl_3N_3OS$, there are four independent molecules in the asymmetric unit; their geometries are the same within experimental error. The six atoms of the thiatriazine ring and the 3,5-chloro atoms are all essentially coplanar.

Comment

As part of our continuing investigations into generating inorganic polymers *via* the ring-opening polymerization of heterocycles (McWilliams *et al.*, 2000; Gates & Manners, 1997; Chivers *et al.*, 1999), we explored the reactivity of the title compound, (II), with various Lewis acids. Compound (II) was prepared by oxidizing the S^{IV} trichlorothiatriazine ring in (I) with a mixture of $KMnO_4$ and $CuSO_4 \cdot xH_2O$ ($x = 4$–6) in CH_2Cl_2 (Chivers *et al.*, 1999).
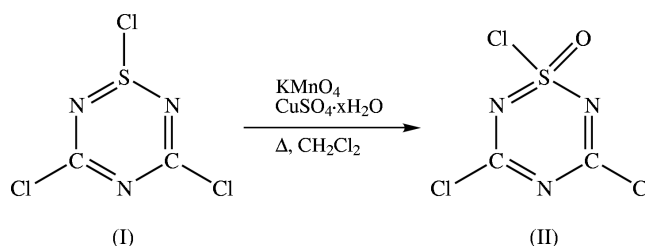
A view of the four independent molecules (named *A, B, C* and *D*) in (II) is shown in Fig. 1, and selected bond lengths and angles are given in Table 1. The geometries of the independent molecules are the same within experimental error. The six atoms of the thiatriazine ring and the 3,5-chloro atoms are all essentially coplanar, with root-mean-square deviations of 0.013, 0.026, 0.044 and 0.061, respectively, for molecules *A, B, C* and *D*. This is in contrast to the structure of compound (I) (Chen *et al.*, 1993), where the three-coordinate S atom deviates significantly (*ca* 0.314 Å) from the plane of the three N and two C atoms in the ring. In addition, compound (I) has significantly elongated S—N bond lengths [in the range 1.615 (1)–1.616 (2) Å] compared to (II), which has distances for the same bonds ranging from 1.5760 (18) to 1.5867 (19) Å. In (II), the S—Cl bond lengths (in molecules *A, B, C,* and *D*) range from 1.9935 (8) to 2.0084 (8) Å, whereas in (I) this distance is slightly longer at 2.132 (1) Å. The differences in bond lengths may be attributed to the higher formal positive charge on the S^{VI} center in (II) compared to that on the S^{IV} center in (I).

Experimental

Compound (II) was prepared in an identical manner to that previously published by Chivers *et al.* (1999). However, upon

sublimation of the crude residue at 298 K onto a cold finger cooled to 253 K, white opaque blocks of (II) were formed.

Crystal data

$C_2Cl_3N_3OS$	$D_x = 2.027$ Mg m^{-3}
$M_r = 220.46$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 19673
$a = 18.6270$ (3) Å	reflections
$b = 7.3160$ (1) Å	$\theta = 2.6–27.5°$
$c = 21.2340$ (5) Å	$\mu = 1.48$ mm^{-1}
$\beta = 93.1840$ (7)°	$T = 150$ (1) K
$V = 2889.20$ (9) Å^3	Block, white
$Z = 16$	$0.43 \times 0.38 \times 0.16$ mm

Data collection

Nonius KappaCCD diffractometer	5166 reflections with $I > 2\sigma(I)$
φ scans and ω scans with κ offsets	$R_{int} = 0.044$
Absorption correction: multi-scan	$\theta_{max} = 27.5°$
(*SORTAV*; Blessing, 1995)	$h = -24 \rightarrow 24$
$T_{min} = 0.681$, $T_{max} = 0.795$	$k = -9 \rightarrow 9$
19673 measured reflections	$l = -20 \rightarrow 27$
6606 independent reflections	

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0235P)^2$
$R[F^2 > 2\sigma(F^2)] = 0.032$	$+ 0.8966P]$
$wR(F^2) = 0.075$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.02$	$(\Delta/\sigma)_{max} = 0.001$
6606 reflections	$\Delta\rho_{max} = 0.38$ e Å^{-3}
362 parameters	$\Delta\rho_{min} = -0.43$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cl2A—S1A	1.9935 (8)	Cl2C—S1C	2.0064 (8)
S1A—O1A	1.4149 (18)	S1C—O1C	1.4155 (17)
S1A—N2A	1.5798 (19)	S1C—N1C	1.579 (2)
S1A—N3A	1.580 (2)	S1C—N2C	1.581 (2)
Cl2B—S1B	2.0084 (8)	Cl2D—S1D	1.9947 (8)
S1B—O1B	1.4154 (16)	S1D—O1D	1.4142 (16)
S1B—N2B	1.5760 (18)	S1D—N2D	1.578 (2)
S1B—N3B	1.5847 (19)	S1D—N3D	1.5867 (19)
N2A—C1A—N1A	130.8 (2)	N3C—C1C—N1C	130.3 (2)
N3A—C2A—N1A	130.6 (2)	N3C—C2C—N2C	130.8 (2)
N2B—C1B—N1B	130.3 (2)	N1D—C1D—N2D	130.9 (2)
N3B—C2B—N1B	130.3 (2)	N3D—C2D—N1D	130.4 (2)

Data collection: *COLLECT* (Nonius, 1997–2002); cell refinement: *DENZO-SMN* (Otwinowski & Minor, 1997); data reduction:
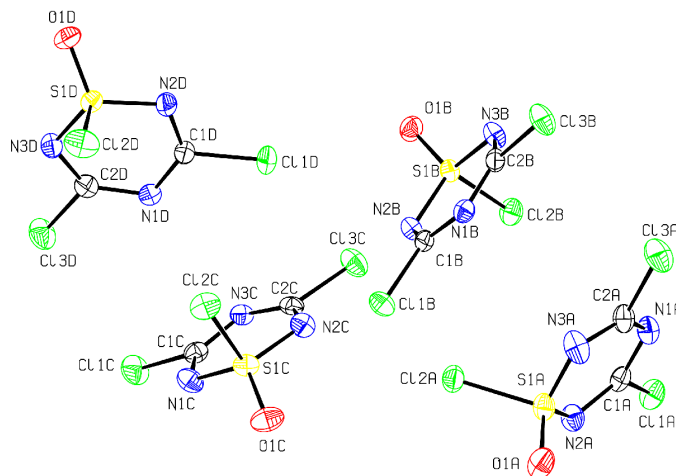
Figure 1
View of the four independent molecules of the title compound, showing the labeling scheme. Displacement ellipsoids are drawn at the 30% probability level.

DENZO-SMN; program(s) used to solve structure: *SHELXTL/PC* (Sheldrick, 2001); program(s) used to refine structure: *SHELXTL/PC*; molecular graphics: *SHELXTL/PC*; software used to prepare material for publication: *SHELXTL/PC*.

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