Discussion. Bond lengths and angles in the acetal group of (I) are closely similar to those of the acetal enol ether described in the preceding paper (Jones *et al.*, 1978), and thus confirm the significance of the deviations from normal C–O bond lengths.

The molecules are linked to form centrosymmetric dimers by typical carboxylic acid H bonding, with non-bonded distances (Å) as follows: O(1)···O(2′) 2·64, O(1)···H(10′) 1·75 (primed atoms at $1-x$, $-y$, $2-z$).

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3,5-Dichloro-4*H*-1,2,6-thiadiazin-4-one

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Abstract. $C_3Cl_2N_2OS$, monoclinic, $P2_1/c$, $a = 7{\cdot}9504\,(5)$, $b = 13{\cdot}2827\,(12)$, $c = 6{\cdot}3390\,(4)$ Å, $\beta = 106{\cdot}350\,(5)°$, $Z = 4$, $D_c = 1{\cdot}89$ g cm^{-3}. The crystal structure has been solved by direct methods and refined by least-squares techniques to $R_w = 5{\cdot}7\%$. The thiadiazine ring is nearly planar.

Introduction. A number of compounds related to the title compound, whose structure is given in Fig. 1, have been studied in the Organic Chemistry Laboratory of this University (Geevers & Trompen, 1974). In order to establish the accurate geometry of these compounds an X-ray structure analysis of $C_3Cl_2N_2OS$ has been carried out.

A crystal suitable for X-ray diffraction experiments (maximum dimension 0·5 mm) was supplied by Dr W. P. Trompen. Cell constants were determined by a least-squares fit of diffraction angles of 41 reflexions, determined accurately on a Philips PW1100 four-circle diffractometer. Intensities were measured using an ω–2θ scan (Mo $K\alpha$ radiation, $\lambda = 0{\cdot}71069$ Å, graphite monochromator, $\theta_{\max} = 30°$). The space group was determined as $P2_1/c$ from the systematic absences $0k0$ for $k = 2n + 1$ and $h0l$ for $l = 2n + 1$. The number of reflexions measured was 2004. 1444 reflexions had $I > 2\sigma(I)$ and were considered to be observed. No systematic change in the intensities of the standard reflexions (measured at intervals of one hour) could be detected. No absorption correction was applied.

The structure was solved by the program *MULTAN* (Germain, Main & Woolfson, 1971). Positions and anisotropic thermal parameters were refined with the *ORFLS* program (Busing, Martin & Levy, 1962). The scattering factors for C, N and O were calculated from Clementi's (1965) wavefunctions (Harkema, 1971).

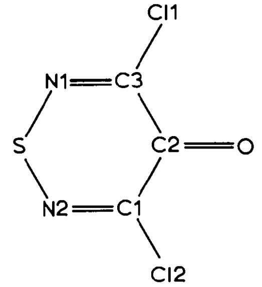

Fig. 1. Atomic arrangement of 3,5-dichloro-4*H*-1,2,6-thiadiazin-4-one.

Table 1. *Positional parameters* (×10⁴)

	x	*y*	*z*
C(1)	94 (4)	1141 (2)	3747 (5)
C(2)	1454 (4)	1504 (2)	5693 (5)
C(3)	3252 (4)	1311 (2)	5563 (6)
N(1)	3699 (3)	915 (2)	3967 (5)
N(2)	323 (3)	710 (2)	2057 (4)
O	1131 (3)	1920 (2)	7231 (4)
Cl(1)	4891 (1)	3342 (1)	2857 (2)
Cl(2)	7965 (1)	1299 (1)	3844 (2)
S	7739 (1)	5515 (1)	3213 (2)

Table 2. *Bond distances* (Å)

C(1)–C(2)	1·474 (5)	C(3)–Cl(1)	1·720 (4)
C(1)–Cl(2)	1·723 (3)	C(3)–N(1)	1·276 (4)
C(1)–N(2)	1·272 (4)	N(1)–S	1·615 (3)
C(2)–C(3)	1·477 (5)	N(2)–S	1·619 (3)
C(2)–O	1·209 (4)		

Table 3. *Bond angles* (°)

N(2)–C(1)–Cl(2)	117·3 (3)	C(2)–C(3)–Cl(1)	114·9 (3)
N(2)–C(1)–C(2)	127·3 (4)	C(2)–C(3)–N(1)	127·3 (4)
Cl(1)–C(1)–C(2)	115·3 (3)	N(1)–C(3)–Cl(1)	117·9 (3)
C(1)–C(2)–C(3)	113·0 (3)	C(3)–N(1)–S	121·8 (3)
C(1)–C(2)–O	123·5 (4)	C(1)–N(2)–S	121·8 (3)
C(3)–C(2)–O	123·6 (4)	N(1)–S–N(2)	108·8 (2)

Table 4. *Distances* (Å) *of the atoms from the best plane fitted to the positions of the atoms in the six-membered ring*

The equation of the plane is

$$2{\cdot}9912x + 38{\cdot}6604y - 9{\cdot}1517z = 1{\cdot}0000.$$

C(1)*	−0·003 (3)	O	−0·044 (3)
C(2)*	−0·012 (3)	Cl(1)	0·098 (1)
C(3)*	0·016 (3)	Cl(2)	0·033 (1)
N(1)*	−0·004 (3)	S*	−0·009 (1)
N(2)*	0·013 (3)		

* Included in mean-plane calculation.

For the S and Cl atoms the scattering factors given by Dawson (1960) were used. The weight of each reflexion was taken to be $w = 1/\sigma^2$. The σ was taken as: $\sigma = 2S + 0{\cdot}01|F_o|$, where S is the standard deviation due to counting statistics and F_o is the observed structure factor. The final weighted R factor was 5·7%. Positional parameters are given in Table 1.* Bond distances and angles are collected in Tables 2 and 3. All reflexions were used in the refinement.

Discussion. The distances of all atoms to the best plane fitted to the positions of the atoms in the thiadiazine ring are given in Table 4. The table shows that the six-membered ring is nearly planar. The deviations of the terminal Cl and O atoms from the plane are, however, significant.

The S–N bonds in the title compound are appreciably longer than the corresponding value in the sulphurdiimine group (–N=S=N–): 1·54 Å (Gieren & Pertlik, 1976; Kops, Van Aken & Schenk, 1973). The bonds in the sulphurdiimine group are considered to be S–N double bonds. The bond lengths found here indicate that the sulphurdiimine group is conjugated with the rest of the molecule. The S–N bonds in the title compound can be compared with the S–N bonds found in 3,4-diphenyl-1,2,5-thiadiazole: 1·636 (4) and 1·630 (4) Å (Mellini & Merlino, 1976). The bonds in the latter compound are considered to have appreciable double-bond character.

The C–N bonds are very short. The values found are close to that expected for a C–N double bond: 1·27 (2) Å (Häfelinger, 1970). The bond lengths in the C–C–C segment indicate some conjugation with the rest of the molecule.

Bond angles in the molecule deviate (in some cases considerably) from the value of 120° expected for sp^2 hybridized atoms.

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* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 33626 (13 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.