thus its occurrence in a small crystal structure may be of considerable interest. Hydrogen-bond distances and angles are given in Table 5.

Table 5. *Hydrogen-bond lengths and angles*

| X | H | Y | X···Y | ∠X···H···Y |
|---|---|---|---|---|
| $N(1)_2^{(i)}$ | $H(N1)_2^{(i)}$ | $O(3)_1^{(ii)}$ | 2·873 (5) Å | 175·5 (2·7)° |
| $O(3)_2^{(i)}$ | $H(N1)_1^{(ii)}$ | $N(1)_1^{(i)}$ | 2·856 (5) | 168·6 (2·9) |
| $N(2)_2^{(i)}$ | $H(N2)_2^{(i)}$ | $O(4)_1^{(i)}$ | 2·937 (4) | 164·6 (2·4) |
| $O(4)_2^{(i)}$ | $H(N2)_1^{(ii)}$ | $N(2)_1^{(ii)}$ | 2·968 (5) | 168·1 (2·8) |

Subscript 1 or 2 refers to molecule 1 or 2 within the asymmetric unit. Superscripts: (i) $x,y,z$. (ii) $\frac{1}{2}-x, -\frac{1}{2}+y, \frac{1}{2}-z$.

I wish to thank the students of the MSc in Biomolecular Organisation (1972/74) at Birkbeck College, who prepared the crystals under the supervision of Dr E. J. Hedgely; also Drs D. S. Moss and P. F. Lindley and Mr A. Gosling for help with computing, and Mr D. Parry for help in the preparation of diagrams.

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# The Crystal Structure of 7-Amino-2*H*,4*H*-*vic*-triazolo[4,5-*c*]-1,2,6-thiadiazine-1,1-dioxide Monohydrate (ATTM)

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The crystal structure of 7-amino-2*H*,4*H*-*vic*-triazolo[4,5-*c*]-1,2,6-thiadiazine-1,1-dioxide monohydrate has been determined by single-crystal X-ray diffraction techniques. The compound crystallizes in the monoclinic system, space group $P2_1/c$ with $a=10·552$ (2), $b=8·509$ (2), $c=8·835$ (2) Å, $\beta=90·34$ (1)° and $Z=4$. Intensity data were collected with a four-circle diffractometer using Mo $K\alpha$ radiation. The crystal structure was solved by a three-dimensional Patterson synthesis and refined by the least-squares method to a final $R$ of 0·055 for 1708 observed reflexions. The packing in the crystal is determined by hydrogen bonds in which all available groups participate. The water molecule has a trigonal coordination.

## Introduction

This compound (hereinafter ATTM) was known to be similar to the previously reported anhydrous analogue (hereinafter ATT) (Foces-Foces, Cano & García-Blanco, 1974), and the present work was undertaken in order to determine the main characteristics of the N–SO$_2$–N group and compare them with those of ATT. Initially, the chemical formula of ATTM was not exactly known. The structure analysis confirmed the formulation $C_3H_4N_6O_2S.H_2O$.

## Experimental

A summary of the crystal data is given in Table 1.

Table 1. *Crystal data*

Standard deviations, given in parentheses refer to the least significant digit.

| | |
|---|---|
| $C_3H_4N_6O_2S.H_2O$ | M.W. 206·06 |
| Space group: $P2_1/c$ | $Z=4$ |
| $\lambda$(Mo $K\bar{\alpha}$) = 0·7107 Å | $V=791·6$ Å$^3$ |
| $a=10·553$ (2) Å | $D_{obs}$(flotation) = 1·69 g cm$^{-3}$ |
| $b=8·509$ (2) Å | $D_{cal}=1·72$ g cm$^{-3}$ |
| $c=8·835$ (2) Å | $F_{000}=424$ |
| $\beta=90·34$ (1)° | $\mu=3·946$ cm$^{-1}$ |

A crystal of approximate dimensions 0·50 × 0·20 × 0·08 mm was mounted on a Philips four-circle single-crystal diffractometer. Intensities were recorded in the $\omega$–$2\theta$ scan mode with $\theta$ between 2° and 30°. Graphite monochromatized Mo $K\alpha$ radiation was used. 2302 reflexions were measured, of which 1708 had intensities greater than twice their standard deviation ($\sigma$), $\sigma$ being calculated from the counting statistics of the measurements. The intensity data were corrected for Lorentz and polarization effects. No absorption correction was applied. Approximate values for the scale factors and the initial overall isotropic thermal parameter $B$ (2·07 Å$^2$) were obtained from a Wilson plot.

### Solution and refinement of the structure

The sulphur atom was located from a three-dimensional Patterson synthesis by means of the Harker peaks. The remaining non-hydrogen atomic positions were obtained by the iterative Fourier technique with an initial set of phases based on the sulphur-atom positions. The $R$ value was 0·24. The structure was refined by the full-matrix least-squares method using anisotropic temperature factors. All hydrogen atoms were located in a difference map and refined. The temperature factors for these atoms were the isotropic ones equivalent to the anisotropic values of the heavy atom to which the hydrogen atoms are bonded (Hamilton, 1959). Weights were assigned according to $w=1/\sigma^2$, where $\sigma=(\sigma_F f(\sin\theta).\sigma_1)$; $\sigma_F^2$ is the variance of $|F_o|$ estimated from the counting statistics; $f(\sin\theta)=0{\cdot}2354/\sin\theta$ and $\sigma_1=2{\cdot}5234$ to give a constant value for $w\Delta^2$, where $\Delta=|F_o-F_c|$. The final $R$ values, weighted $R_w=(\sum w\Delta^2/\sum w|F_o|^2)^{1/2}$ and unweighted, respectively, were 0·055 and 0·049. A final difference synthesis had no peaks greater than 0·46 e Å$^{-3}$. The atomic scattering factors for all atoms were taken from *International Tables for X-ray Crystallography* (1962).

The values of positional and thermal parameters together with their standard deviations are given in Tables 2 and 3.*

Table 2. *Final atomic coordinates*

The least-squares e.s.d.'s given in parentheses refer to the last digits.

| | $x$ | $y$ | $z$ |
|---|---|---|---|
| N(1) | 0·3445 (3) | 0·8810 (3) | 0·4110 (4) |
| N(2) | 0·2596 (3) | 0·9232 (4) | 0·5119 (4) |
| N(3) | 0·1975 (3) | 0·8092 (4) | 0·5834 (4) |
| N(4) | 0·2224 (4) | 0·5273 (4) | 0·5598 (4) |
| S(5) | 0·2568 (1) | 0·3988 (1) | 0·4278 (1) |
| O(5*a*) | 0·1590 (3) | 0·3961 (4) | 0·3148 (3) |
| O(5*b*) | 0·2801 (3) | 0·2521 (3) | 0·5028 (4) |
| N(6) | 0·3859 (3) | 0·4569 (3) | 0·3530 (4) |
| C(7) | 0·4120 (3) | 0·6087 (4) | 0·3347 (4) |
| C(8) | 0·3387 (3) | 0·7230 (4) | 0·4158 (4) |
| C(9) | 0·2488 (4) | 0·6813 (4) | 0·5230 (4) |
| N(10) | 0·5057 (4) | 0·6501 (4) | 0·2460 (5) |
| O(*w*) | 0·0605 (4) | 0·0841 (7) | 0·2654 (7) |
| H(2) | 0·2545 (53) | 1·0086 (70) | 0·5385 (64) |
| H(4) | 0·1735 (63) | 0·5086 (82) | 0·6369 (76) |
| H(10*a*) | 0·5407 (51) | 0·5826 (69) | 0·1966 (62) |
| H(10*b*) | 0·5286 (58) | 0·7386 (81) | 0·2539 (71) |
| H(*w*1) | 0·0870 (76) | 0·1866 (105) | 0·3213 (97) |
| H(*w*2) | 0·0216 (85) | 0·0743 (117) | 0·3181 (100) |

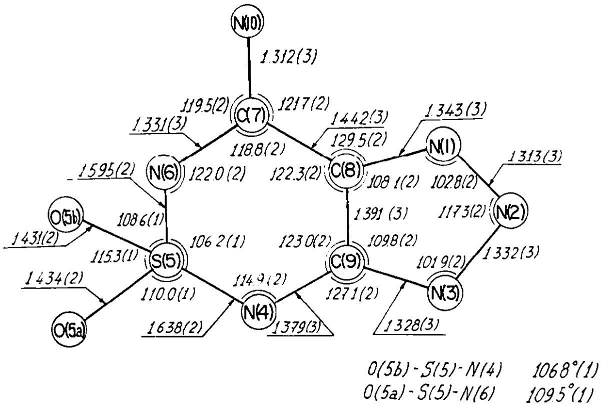

Fig. 1. Bond lengths (Å), valence angles (°) with their estimated standard deviations referred to the last significant digits.

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* A list of structure factors has been deposited with the British Library Lending Division as Supplementary Publication No. SUP 31004 (11 pp., 1 microfiche). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

Table 3. *Thermal parameters* ($\times 10^4$) *for the heavy atoms, given according to the expression exp* ($-2\pi^2\sum U_{ij}a_i^*a_j^*h_ih_j$)

The hydrogen thermal parameters are the equivalent isotropic temperature factors of the corresponding heavy atoms. The least-squares e.s.d.'s are given in parentheses referring to the last digits.

| | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{12}$ | $U_{13}$ | $U_{23}$ |
|---|---|---|---|---|---|---|
| N(1) | 345 (16) | 159 (13) | 350 (17) | −4 (13) | 77 (13) | 1 (12) |
| N(2) | 406 (19) | 125 (14) | 392 (19) | 4 (12) | 109 (15) | −33 (12) |
| N(3) | 403 (18) | 169 (14) | 391 (19) | −10 (13) | 136 (15) | −24 (13) |
| N(4) | 557 (23) | 152 (14) | 398 (20) | −46 (15) | 238 (18) | −16 (14) |
| S(5) | 312 (4) | 102 (3) | 307 (4) | −14 (3) | 74 (3) | −7 (3) |
| O(5*a*) | 370 (15) | 327 (15) | 445 (17) | −28 (13) | −42 (13) | −30 (14) |
| O(5*b*) | 520 (19) | 143 (12) | 510 (19) | −15 (12) | 87 (14) | 63 (12) |
| N(6) | 335 (16) | 133 (12) | 365 (18) | 14 (12) | 127 (14) | −1 (12) |
| C(7) | 262 (16) | 171 (14) | 280 (17) | 4 (14) | 21 (13) | −10 (14) |
| C(8) | 301 (18) | 144 (15) | 253 (17) | 0 (13) | 46 (14) | 6 (13) |
| C(9) | 344 (19) | 144 (15) | 284 (17) | −7 (14) | 75 (15) | −17 (13) |
| N(10) | 352 (17) | 174 (14) | 446 (19) | −22 (13) | 155 (14) | −18 (13) |
| O(*w*) | 535 (25) | 778 (33) | 1255 (46) | −240 (23) | 488 (28) | −570 (32) |

Hydrogen atom $U$ values ($\times 10^4$)

| H(2) | H(4) | H(10*a*) | H(10*b*) | H(*w*1) | H(*w*2) |
|---|---|---|---|---|---|
| 247 (155) | 283 (205) | 212 (148) | 373 (113) | 765 (292) | 542 (346) |

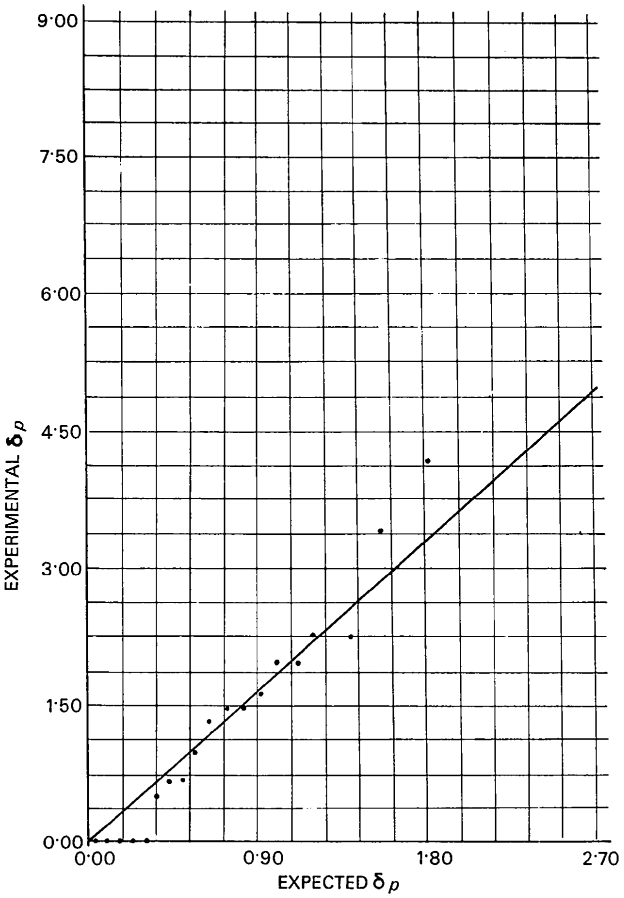

Fig. 2. Half-normal δp probability plot for all bond distances for ATT and ATTM compounds.

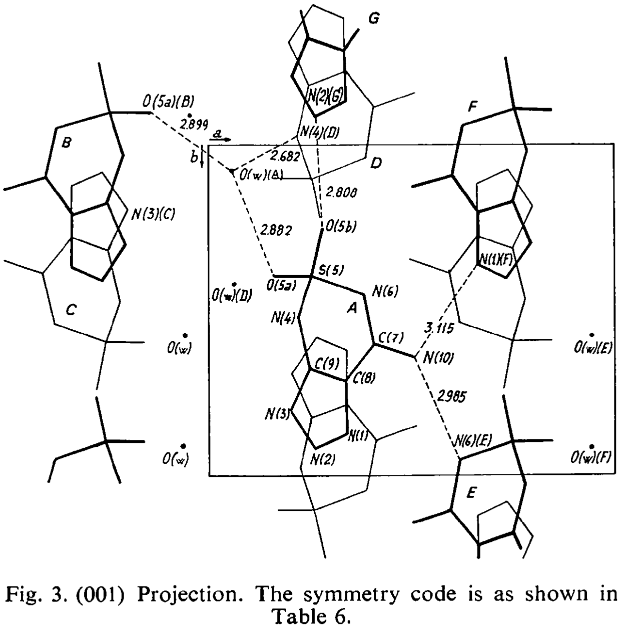

Fig. 3. (001) Projection. The symmetry code is as shown in Table 6.

## Discussion of the structure

All intramolecular distances and angles, together with their standard deviations, are shown in Fig. 1. Table 5 shows a list of torsional angles (Klyne & Prelog, 1960) in the thiadiazine ring.

The arrangement of bonds about the sulphur atom is a distorted tetrahedron, the O(5*a*)–S(5)–O(5*b*) angle of 115·3° being greater than the rest (Fig. 1) and significantly different from the tetrahedral angle. The N–N, O–O and N–O distances in the N–$SO_2$–N group vary between the values of 2·419(4) and 2·585(4) Å. The two S–O bond lengths of 1·431 and 1·434 Å are approximately equal to those found in other sulphones (~1·43 Å).

Planarities of three sections of the molecule have been considered: (1) the atoms of the $SO_2$ group, (2) the thiadiazine ring, excluding S(5), and (3) the five-membered ring. The least-squares planes referred to orthogonal axes are given in Table 4. The sections (2) and (3) were found to be planar, the maximum deviations of atoms being 0·026 and 0·003 Å, respectively. The deviation of the sulphur atom from plane (2) is −0·528 Å; O(5*b*) shows a small deviation from the same plane.

Table 4. *Deviations of the atoms from some least-squares planes in the molecule, with their dihedral angles*

The equations of the planes are in the form $AX+BY+CZ+D=0$, where $X, Y, Z$ are coordinates referred to the orthogonal axes.

(* denotes the atoms used in the plane calculations).

| Plane 1 | | Plane 2 | | Plane 3 | |
|---|---|---|---|---|---|
| S(5) | 0·0* | N(4) | 0·024 * | N(1) | 0·001* |
| O(5*a*) | 0·0* | S(5) | −0·528 | N(2) | 0·002* |
| O(5*b*) | 0·0* | O(5*a*) | −1·959 | N(3) | −0·004* |
| | | O(5*b*) | 0·117 | S(5) | −0·503 |
| | | N(6) | −0·032* | O(5*b*) | 0·148 |
| | | C(7) | 0·040* | O(5*a*) | −1·934 |
| | | C(8) | −0·015* | C(8) | −0·004* |
| | | C(9) | −0·017* | C(9) | 0·005* |
| | | N(10) | 0·185 | | |

Plane 1: $-0{\cdot}6783X+0{\cdot}2389Y+0{\cdot}6994Z+1{\cdot}6172=0{\cdot}0$
Plane 2: $0{\cdot}7067X-0{\cdot}0064Y+0{\cdot}7075Z+5{\cdot}0728=0{\cdot}0$
Plane 3: $0{\cdot}7014X-0{\cdot}0095Y+0{\cdot}7126Z+5{\cdot}0427=0{\cdot}0$

∠(Plane 1) (Plane 2) 89·4°
∠(Plane 2) (Plane 3) 0·5°

Table 5. *Twist angles*

| | |
|---|---|
| S(5)–N(6)–C(7)–C(8) | 15·77° |
| C(8)–C(9)–N(4)–S(5) | −23·86 |
| N(6)–C(7)–C(8)–C(9) | 6·06 |
| C(7)–C(8)–C(9)–N(4) | −0·49 |
| C(9)–N(4)–S(5)–N(6) | 38·38 |
| N(4)–S(5)–N(6)–C(7) | −35·87 |

Several half normal probability plots (Abrahams & Keve, 1971) were calculated in order to compare the structure of ATTM with that of the previously reported ATT (Foces-Foces *et al.*, 1975). Using all the

Table 6. *Hydrogen bonds, and short* X–H···Y *van der Waals contacts*

Distances are in Å and angles in degrees, with the e.s.d.'s from least squares in parentheses.

| | | | Distances | | | Angles | | |
|---|---|---|---|---|---|---|---|---|
| X | H | Y | X···Y | X–H | H···Y | X–H···Y | H–X···Y | X···Y···H |
| N(2) (*G*) | H(2) (*G*) | O(5*b*) (*A*) | 2·808 (3) | 0·817 (44) | 2·044 (44) | 155·3 (42) | 17·7 (30) | 7·0 (12) |
| N(4) (*D*) | H(4) (*D*) | O(*w*) (*A*) | 2·682 (5) | 0·854 (48) | 1·845 (48) | 165·3 (46) | 10·1 (32) | 4·6 (15) |
| O(*w*) (*A*) | H(*w*1) (*A*) | O(5*a*) (*A*) | 2·892 (4) | 0·915 (72) | 2·017 (69) | 159·5 (57) | 14·2 (39) | 6·4 (19) |
| O(*w*) (*A*) | H(*w*2) (*A*) | O(5*a*) (*B*) | 2·899 (4) | 0·934 (65) | 2·343 (67) | 117·8 (53) | 45·6 (43) | 16·5 (16) |
| O(*w*) (*A*) | H(*w*3) (*A*) | N(3) (*C*) | 3·175 (4) | 1·204 (83) | 3·193 (80) | 78·3 (39) | 79·9 (36) | 21·8 (14) |
| N(10) (*A*) | H(10*a*) (*A*) | N(1) (*F*) | 3·115 (3) | 0·821 (46) | 2·297 (47) | 174·4 (45) | 4·1 (33) | 1·5 (12) |
| N(10) (*A*) | H(10*b*) (*A*) | N(6) (*E*) | 2·985 (3) | 0·893 (47) | 2·137 (47) | 158·3 (41) | 15·4 (29) | 6·4 (12) |

Symmetry code

| | | | |
|---|---|---|---|
| (*A*) | $x$ | $y$ | $z$ |
| (*B*) | $-x$ | $-\frac{1}{2}+y$ | $\frac{1}{2}-z$ |
| (*C*) | $-x$ | $1-y$ | $1-z$ |
| (*D*) | $x$ | $\frac{1}{2}-y$ | $-\frac{1}{2}+z$ |
| (*E*) | $1-x$ | $\frac{1}{2}+y$ | $\frac{1}{2}-z$ |
| (*F*) | $1-x$ | $-\frac{1}{2}+y$ | $\frac{1}{2}-z$ |
| *G*) | $x$ | $-1+y$ | $z$ |

distances, the plot (Fig. 2) is quite linear, suggesting that the e.s.d.'s have been underestimated by a factor of only about 1·7. The main departures are due to the S(5)–N(4) and N(2)–N(3) distances. The second plot was made using all the bond angles and showed a bias corresponding mainly to the hydrogen atoms. The remaining bond angles gave a quite linear plot with a slope of 3·0 and main departures in the O(5*a*)–S(5)–N(4) and S(5)–N(4)–C(9) angles.

There is as yet no theory which accounts satisfactorily for the bond lengths in all the oxy compounds of sulphur (Truter, 1962). The simplest examination of compounds in which sulphur(II) (IV,VI) has 2 (3,4) neighbours, respectively, shows that they are all based on an $sp^3$-hybridization. This gives two lone pairs of electrons in sulphur(II), one lone pair and one electron in the *d* orbitals in neutral compounds of sulphur(IV), and two electrons in the *d* orbitals of sulphur(VI). Cruickshank's (1961) discussion of X–O bonds is restricted to molecules in which the X (Si,P,S,Cl) atoms are tetrahedrally coordinated. In any molecule in which sulphur is surrounded by four ligands in an approximately tetrahedral arrangement, $\pi$ bonding can occur between suitable ligand orbitals and the *d*-sulphur orbitals. Cruickshank finds a linear relationship between S–O bond length and $\pi$-bond order, when only oxygen atoms are bonded to the sulphur atoms. The effective nuclear charge, $Z_{\text{eff}}(3d)$, for the 3*d* orbitals is altered and this is reflected in a lengthening of the S–O bonds, when the other atoms are less electronegative than oxygen. The relatively small contraction of the S–O distances (1·3 Å for $\pi$-bond order 1) may be ascribed to the smaller electronegativity of the nitrogen atoms compared with the oxygen atoms and to the asymmetry of the bonding around sulphur.

For the present compound (ATTM), as well as for the previously reported ATT (Foces-Foces, Cano & García-Blanco, 1975), the lone pair on the nitrogen atoms of the N–$SO_2$–N group and the $\pi$-bond order of $\frac{4}{5}$, suggested by the Cruickshank relationship for the S–O bonds, could explain the shortening of the S–N distances mentioned above.

In both compounds there also exists a significant difference between the two S–N distances which might be due to the same effect which causes a change in electronegativity of the carbon atom with its state of hybridization (Dewar, 1969). N(6) is partially double bonded to C(3) while N(4) is bonded to three different atoms implying smaller electronegativity, and so giving a S(5)–N(4) distance greater than S(5)–N(6), with greater electronegativity for N(6).

## The molecular packing and hydrogen bonding

The packing in the crystal involves the formation of hydrogen bonds in which the water molecule plays a dominant role (Fig. 3). The shortest intermolecular contacts and angles including hydrogen bonds are listed in Table 6.

Around N(10) there are two short contacts which relate the H atoms to N(1) and N(6) in molecules *F* and *E* respectively. The $NH_2$ plane forms an angle of 9° with the thiadiazine ring.

The hydrogen atom in the five-membered ring was found to be attached to N(2), as in ATT (Foces-Foces *et al.*, 1975) and an intermolecular contact N(2)(*G*)··· O(5*b*) of 2·808 Å was found.

From Table 6 it can be seen that these contacts have a reasonable geometry (Donohue & Hamilton, 1968).

The water molecule, with an angle H(*w*1)–O(*w*)–H(*w*2) of 92°, has three close contacts (of type O–H···O) of 2·899 and 2·892 Å respectively, and one N–H···O contact of 2·682 Å. The first can be considered as a weak interaction since the O–H···O angle (117·8°) is unfavourable. N(4)(*D*) is a hydrogen-bond donor while O(5*a*)(*A*) and O(5*a*)(*B*) are acceptors of O(*w*) (Fig. 3).

There exists an intermolecular contact of 3·175 Å between O(*w*) and N(3)(*C*). A high peak in the difference synthesis was found between these atoms, but the hydrogen-bonding geometry around this hypothetical H(*w*3) atom was very poor (Table 6). An attempt at refinement including all hydrogen atoms gave the highest e.s.d.'s for the H(*w*3) atom. Moreover, we found that the H(4)(*D*)···H(*w*3) (*A*) distance is quite close to the minimum H···H van der Waals distance of 2·4 Å (Pauling, 1960). Therefore the existence of the H($w$3) atom would lead to an unacceptable crowding of hydrogen atoms about O($w$) and, as well, the O($w$)···N(3) intermolecular contact is greater than the minimum van der Waals N···O contact of 2·9 Å (Pauling, 1960).

## Thermal motion

The magnitudes and angles of the principal axes of thermal motion as derived from the parameters of Table 3 are listed in Table 7, referred to an orthonormal system of axes oriented as follows: $X$ axis along **a**, $Y$ axis along **b** and $Z$ axis along **c***. The maximum r.m.s. displacements for all atoms have been found to be quasiperpendicular to the mean planes in the molecule (planes 2 and 3 in Table 4). The average angle (not given on Table 7) between these planes and the direction of maximum r.m.s. displacements is 9° (excluding the angle corresponding to the O(5$a$) atom which is 65°).

Table 7. *Root mean square* (*r.m.s.*) *components of thermal vibrations along three principal axes and angles between these and the cell axes*

| | Principal axis | R.m.s. component | Angles with cell axes | | |
|---|---|---|---|---|---|
| | | | 1 | 2 | 3 |
| N(1) | 1 | 0·128 Å | 91° | 179° | 91° |
| | 2 | 0·165 | 50 | 2 | 140 |
| | 3 | 0·203 | 140 | 89 | 130 |
| N(2) | 1 | 0·128 | 92 | 5 | 86 |
| | 2 | 0·165 | 46 | 86 | 135 |
| | 3 | 0·218 | 45 | 92 | 46 |
| N(3) | 1 | 0·135 | 93 | 10 | 81 |
| | 2 | 0·166 | 40 | 81 | 131 |
| | 3 | 0·231 | 48 | 95 | 43 |
| N(4) | 1 | 0·115 | 86 | 4 | 88 |
| | 2 | 0·161 | 128 | 90 | 38 |
| | 3 | 0·260 | 38 | 94 | 53 |
| S(5) | 1 | 0·108 | 87 | 3 | 89 |
| | 2 | 0·161 | 45 | 92 | 135 |
| | 3 | 0·201 | 45 | 93 | 45 |
| O(5$a$) | 1 | 0·174 | 107 | 155 | 108 |
| | 2 | 0·191 | 26 | 112 | 76 |
| | 3 | 0·219 | 109 | 102 | 23 |
| O(5$b$) | 1 | 0·109 | 86 | 10 | 99 |
| | 2 | 0·208 | 48 | 100 | 136 |
| | 3 | 0·245 | 43 | 87 | 48 |
| N(6) | 1 | 0·118 | 90 | 0 | 90 |
| | 2 | 0·154 | 44 | 90 | 134 |
| | 3 | 0·214 | 46 | 90 | 44 |
| C(7) | 1 | 0·135 | 100 | 13 | 82 |
| | 2 | 0·163 | 34 | 77 | 121 |
| | 3 | 0·176 | 58 | 91 | 32 |
| C(8) | 1 | 0·124 | 92 | 178 | 90 |
| | 2 | 0·159 | 72 | 91 | 162 |
| | 3 | 0·185 | 18 | 91 | 72 |
| C(9) | 1 | 0·122 | 93 | 12 | 78 |
| | 2 | 0·157 | 126 | 101 | 38 |
| | 3 | 0·203 | 36 | 94 | 54 |
| N(10) | 1 | 0·143 | 67 | 28 | 104 |
| | 2 | 0·160 | 45 | 118 | 123 |
| | 3 | 0·225 | 54 | 92 | 36 |
| O($w$) | 1 | 0·177 | 150 | 83 | 61 |
| | 2 | 0·213 | 111 | 147 | 114 |
| | 3 | 0·398 | 69 | 122 | 40 |

## Conclusions

From the crystallographic studies of ATT and ATTM the thiadiazine ring has been shown to have an envelope conformation at the sulphur atom (Table 5). The partial double-bond character of the S–N distances can be explained in term of $\pi$-bonding between the sulphur 3$d$ orbitals and the lone pair of electrons available on the nitrogen atom. The arrangement of bonds around the sulphur atom is a distorted tetrahedron with the O–S–O angle significantly greater than the other angles around the sulphur. The difference between the two S–N distances can be ascribed to the different electronegativities of the two nitrogen atoms.

All the calculations were performed with the crystallographic programs of the X-RAY 70 System on the 1108 UNIVAC computer of the Centro de Procesos de Datos del Ministerio de Educación y Ciencia (Madrid, Spain).

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