Crystal and Molecular Structure of Silver Sulphadiazine (N^1-Pyrimidin-2-ylsulphanilamide)

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The *X*-ray crystal structure analysis of the 1 : 1 title complex is reported. Crystals are monoclinic, space group $P2_1/c$, with a = 6.172(5), b = 9.605(8), c = 20.33(2) Å, β = 96.60(8)°, and Z = 4. The structure has been solved from visually estimated data by the heavy-atom method, and refined by least-squares to R 10.2% for 1 865 non-zero observed reflections. Each silver atom is co-ordinated to three sulphadiazine molecules by a distorted tetrahedral configuration of three nitrogen atoms and one oxygen atom, with Ag–N 2.24, 2.24, and 2.44, and Ag–O 2.52 Å. The molecules are also linked by sheets of NH · · · OS hydrogen bonds as in related sulphonamide structures.

SULPHONAMIDES have been extensively used in medicine for their antibacterial properties, and inorganic silver salts have gained popularity for the control of infections in extensive burns. Compounds formed between silver and sulphonamides have been reported[1] and preparations containing silver sulphadiazine have been used[2] for burn treatment.

The mode of antibacterial action of the title compound

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[1] M. Wruble, *J. Amer. Pharm. Assoc. Sci. Ed.*, 1943, **32**, 80.

[2] C. L. Fox, jun., *Arch. Surg.*, 1968, **96**, 184.

is different from that of the sulphonamides,[3] and *in vitro* silver sulphadiazine appears to interact with deoxyribonucleic acid (DNA),[3-5] thus binding the silver. Silver sulphadiazine is not light-sensitive and unlike silver nitrate does not remove chloride ion from body fluids.[2]

Recently Sandmann *et al.*[6] have characterised silver sulphadiazine and related compounds, concluding that silver is ionically bound to the amide nitrogen atom, and that oxygen atoms are not co-ordinated to the silver ion. Fox[7] had previously reported that the structure of silver sulphadiazine was analogous to the silver ammines.

TABLE 1

Final atomic co-ordinates and thermal * parameters ($\times 10^4$, $B_{\text{iso}} \times 10^2$), with estimated standard deviations in parentheses

Atom	x/a	y/b	z/c	B_{iso}	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
Ag	8 416(2)	6 027(1)	4 718(1)	161(2)	103(4)	38(2)	12(1)	3(8)	9(2)	3(1)
S	4 024(6)	4 032(3)	3 933(2)	103(5)	85(6)	22(1)	6(1)	23(13)	−5(2)	0(1)
O(1)	3 075(17)	2 667(9)	4 000(5)	150(15)	166(16)	17(5)	15(1)	−39(13)	−9(6)	−6(3)
O(2)	6 425(17)	4 073(9)	4 055(5)	136(15)	100(17)	50(5)	6(1)	46(12)	−5(6)	−8(3)
N(1)	2 774(18)	5 011(11)	4 404(5)	109(16)	102(18)	23(5)	8(1)	−38(14)	10(6)	−10(4)
C(1)	3 048(20)	6 485(12)	4 357(6)	77(17)	74(20)	12(5)	6(1)	19(15)	−5(7)	−1(4)
N(2)	4 948(21)	7 014(13)	4 221(6)	192(19)	120(21)	46(7)	14(1)	2(15)	−4(8)	−3(5)
C(3)	4 996(23)	8 399(13)	4 160(6)	135(19)	101(20)	30(6)	12(1)	−42(15)	−29(8)	12(5)
C(4)	3 291(26)	9 248(15)	4 300(9)	255(28)	193(30)	43(9)	14(1)	16(20)	−5(11)	−2(6)
C(5)	1 514(26)	8 588(14)	4 479(7)	164(22)	124(24)	23(7)	21(2)	32(20)	−1(9)	−4(5)
N(6)	1 350(18)	7 212(10)	4 482(5)	87(15)	84(15)	10(5)	10(1)	38(13)	−6(6)	−8(3)
C(7)	3 348(25)	4 604(14)	3 148(7)	163(21)	130(24)	43(7)	10(1)	−42(18)	35(7)	−23(5)
C(8)	4 804(28)	5 344(16)	2 791(8)	217(25)	126(22)	74(8)	15(1)	−20(20)	0(10)	6(6)
C(9)	4 163(28)	5 840(15)	2 164(8)	204(25)	209(26)	58(8)	6(1)	−63(20)	−22(8)	18(5)
C(10)	2 068(23)	5 797(12)	1 871(6)	99(18)	124(22)	26(5)	4(1)	2(15)	5(7)	3(4)
C(11)	0 474(29)	5 081(18)	2 211(9)	295(30)	117(30)	98(10)	16(2)	8(20)	6(9)	14(8)
C(12)	1 163(29)	4 485(19)	2 863(8)	263(28)	169(30)	93(9)	18(2)	−3(20)	31(11)	−2(7)
N(13)	1 428(23)	6 336(14)	1 249(6)	202(21)	190(23)	75(6)	8(1)	32(17)	12(8)	5(5)

* Anisotropic Temperature Factors ($\times 10^4$) defined by: $\exp - (\beta_{11}h^2 + \beta_{22}k^2 + \beta_{33}l^2 + \beta_{12}hk + \beta_{13}hl + \beta_{23}kl)$.

The properties of silver sulphadiazine indicate that it is not a purely ionic species, but other experiments[8] have produced results different from those reported by Fox.[7] It is likely that the various nitrogen or oxygen atoms of the sulphadiazine co-ordinate with the silver atom in some way. Indeed two- and four-co-ordinate silver complexes with electron-donors are well known,[9-16] exhibiting linear or tetrahedral geometry respectively.

We now report the *X*-ray crystal and molecular structure of silver sulphadiazine.

EXPERIMENTAL

Irregular, brittle, plate-like crystals elongated along [100] were prepared by slow evaporation from a 10% ammonia solution at room temperature in the dark. Chemical analysis showed ammonia absent from the complex (Found Ag, 30.1; Sulphadiazine, 69.8. Calc. for 1 : 1 complex Ag, 30.2; Sulphadiazine, 69.8%).

Crystal Data.—$C_{10}H_9AgN_4O_2S$, $M = 357.14$, Monoclinic, $a = 6.172(5)$, $b = 9.605(8)$, $c = 20.33(2)$ Å, $\beta = 96.60(8)°$, $U = 1\,197$ Å^3, $D_m = 1.97$, $D_c = 1.98$ g cm^{-3}, $Z = 4$, $F(000) = 704$. Space group $P2_1/c$ (C_{2h}^5, No. 14). Cu-K_α radiation, $\lambda = 1.5418$ Å; μ(Cu-K_α) = 157 cm^{-1}.

Space-group and unit-cell dimensions were determined by use of Stoë precession-retigraph and Weissenberg cameras. Two crystals were used for data collection, one $0.2 \times 0.1 \times 0.15$ mm for 0—$7kl$, and the other $0.2 \times 0.15 \times 0.15$ mm for $h0$—$3l$. Visually estimated intensity data, from multiple-film equi-inclination Weissenberg photographs, were corrected for Lorentz and polarisation effects, but not for absorption. The standard deviations of the observed structure factors averaged 15% for moderate intensities and 20% for stronger and weaker intensities. Of the 2 740 independent reflections, 2 285 were observed, of which 1 865 had measurable intensities.

Structure Solution and Refinement.—The structure was determined by the heavy-atom method. Partial Fourier syntheses of electron density, phased on the silver positions from a Patterson synthesis, revealed all non-hydrogen atom positions. Structure refinement was by least-squares using the block-diagonal approximation and weighting scheme $\sqrt{w} = F^*/F_0$ for $|F_0| > F^*$ and $\sqrt{w} = F_0/F^*$ for $|F_0| < F^*$ with $F^* = 30$ electrons; 42 low-angle high-intensity reflections were modified for secondary extinction.[17] Unobserved reflections, after Dunning and Vand,[18] were computed throughout but excluded from the refinement. Hydrogen atoms were later introduced at calculated positions (assuming C–H 1.05 Å) but were not refined. Four cycles of isotropic and two of anisotropic

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[3] C. L. Fox, jun., B. W. Rappole, B. W. Stanford, and W. Stanford, *Surgery, Gynaecology, and Obstetrics*, 1969, **128**, 1021.

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[16] C. J. Anti and B. K. S. Lundberg, *Acta Chem. Scand.*, 1971, **25**, 1758.

[17] R. W. James, 'The Crystalline State,' vol. II, Bell, London, 1965.

[18] A. J. Dunning and B. E. Vand, *Acta Cryst.*, 1969, **15**, 1092.

refinement gave a final R of 10.2%. Final parameter shifts were $\leqslant 0.1\sigma$. Table 1 lists final atomic co-ordinates and thermal parameters. Final observed and calculated structure factors are listed in Supplementary Publication No. SUP 21344 (10 pp., 1 microfiche).*

DISCUSSION

The Molecular Structure.—The unit cell is shown in Figure 1, and Figure 2 shows the structure together with the silver co-ordination, and the N–H · · · OS hydrogen bonding in the region $c = \frac{1}{2}$. Table 2(a) lists intermolecular contact distances and angles. The silver atoms and pyrimidine planes coincide approximately

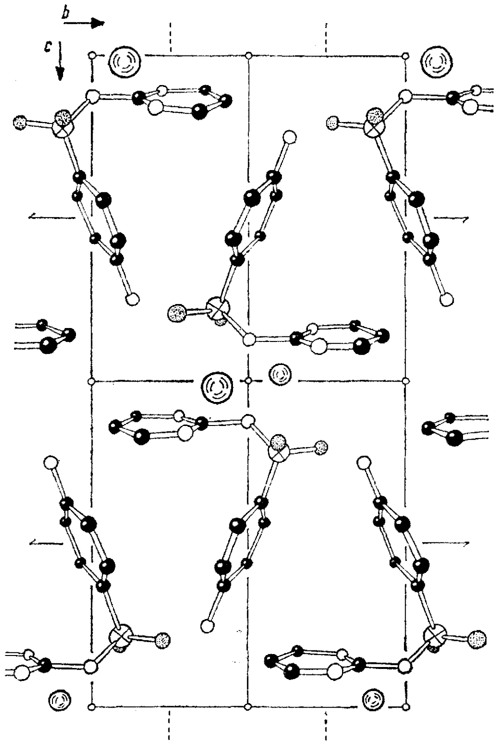

FIGURE 1 Unit cell of silver sulphadiazine (a axis away from reader); large circles Ag, crossed circle S, closed circle C, small open circle N, dotted circle O

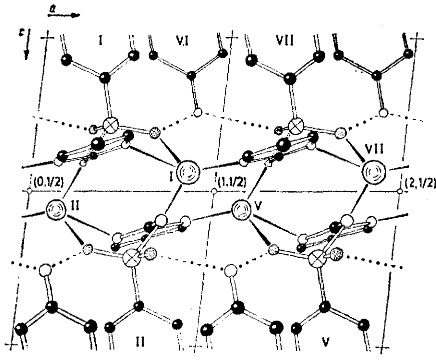

FIGURE 2 Structure of silver sulphadiazine in the region $c = \frac{1}{2}$ viewed down the b axis, illustrating the silver co-ordination (full lines), and the N–H · · · OS hydrogen bonding (shown by dashed lines)

TABLE 2

(a) Intermolecular contacts,* distances (Å), and angles (deg.) with estimated standard deviations in parentheses

(i) Ag–X distances

Ag$^{\mathrm{I}}$–N(6$^{\mathrm{VII}}$)	2.24(1)	Ag$^{\mathrm{I}}$–N(2$^{\mathrm{I}}$)	2.45(1)
Ag$^{\mathrm{I}}$–N(1$^{\mathrm{II}}$)	2.24(1)	Ag$^{\mathrm{I}}$–O(2$^{\mathrm{I}}$)	2.54(1)

(ii) H-bond distances

O(2$^{\mathrm{I}}$) · · · N(13$^{\mathrm{VI}}$)	3.04(2)	O(1$^{\mathrm{VII}}$) · · · N(13$^{\mathrm{VI}}$)	3.05(2)

(iii) H-bond angles

S$^{\mathrm{I}}$–O(2$^{\mathrm{I}}$) · · · N(13$^{\mathrm{VI}}$)	113(1)
S$^{\mathrm{VII}}$–O(1$^{\mathrm{VII}}$) · · · N(13$^{\mathrm{VI}}$)	137(1)
C(10$^{\mathrm{VI}}$)–N(13$^{\mathrm{VI}}$) · · · O(1$^{\mathrm{VII}}$)	118(1)
C(10$^{\mathrm{VI}}$)–N(13$^{\mathrm{VI}}$) · · · O(2$^{\mathrm{I}}$)	115(1)

(iv) X–Ag–X angles

N(1$^{\mathrm{II}}$)–Ag$^{\mathrm{I}}$–N(2$^{\mathrm{I}}$)	99(1)	N(1$^{\mathrm{II}}$)–Ag$^{\mathrm{I}}$–O(2$^{\mathrm{I}}$)	85(1)
N(2$^{\mathrm{II}}$)–Ag$^{\mathrm{I}}$–O(2$^{\mathrm{I}}$)	74(1)	N(1$^{\mathrm{II}}$)–Ag$^{\mathrm{I}}$–N(6$^{\mathrm{VII}}$)	138(1)
O(2$^{\mathrm{I}}$)–Ag$^{\mathrm{I}}$–N(6$^{\mathrm{VII}}$)	128(1)	N(2$^{\mathrm{I}}$)–Ag$^{\mathrm{I}}$–N(6$^{\mathrm{VII}}$)	114(1)

(v) Ag–X–X angles

Ag$^{\mathrm{I}}$–N(2$^{\mathrm{I}}$)–C(1$^{\mathrm{I}}$)	121(1)	Ag$^{\mathrm{I}}$–N(1$^{\mathrm{II}}$)–S$^{\mathrm{II}}$	116(1)
Ag$^{\mathrm{I}}$–N(2$^{\mathrm{I}}$)–C(3$^{\mathrm{I}}$)	113(1)	Ag$^{\mathrm{I}}$–N(1$^{\mathrm{II}}$)–C(1$^{\mathrm{II}}$)	123(1)
Ag$^{\mathrm{I}}$–N(6$^{\mathrm{VII}}$)–C(1$^{\mathrm{VII}}$)	117(1)	Ag$^{\mathrm{I}}$–O(2$^{\mathrm{I}}$)–S$^{\mathrm{I}}$	122(1)
Ag$^{\mathrm{I}}$–N(6$^{\mathrm{VII}}$)–C(5$^{\mathrm{VII}}$)	125(1)		

(vi) Other short contacts <3.8 Å

Ag–X

Ag$^{\mathrm{I}}$–Ag$^{\mathrm{V}}$	2.916(2)	Ag$^{\mathrm{I}}$–C(1$^{\mathrm{II}}$)	3.24(1)
Ag$^{\mathrm{I}}$–N(1$^{\mathrm{VII}}$)	3.00(1)	Ag$^{\mathrm{I}}$–S$^{\mathrm{II}}$	3.277(3)
Ag$^{\mathrm{I}}$–C(1$^{\mathrm{VII}}$)	3.06(1)	Ag$^{\mathrm{I}}$–C(1$^{\mathrm{I}}$)	3.34(1)
Ag$^{\mathrm{I}}$–O(1$^{\mathrm{II}}$)	3.12(1)	Ag$^{\mathrm{I}}$–N(6$^{\mathrm{II}}$)	3.51(1)
Ag$^{\mathrm{I}}$–C(5$^{\mathrm{VII}}$)	3.20(1)	Ag$^{\mathrm{I}}$–S$^{\mathrm{I}}$	3.547(4)
Ag$^{\mathrm{I}}$–C(3$^{\mathrm{I}}$)	3.22(1)	Ag$^{\mathrm{I}}$–N(1$^{\mathrm{I}}$)	3.60(1)

Others

N(1$^{\mathrm{I}}$)–O(2$^{\mathrm{II}}$)	3.23(1)	C(9$^{\mathrm{I}}$)–C(3$^{\mathrm{VI}}$)	3.66(2)
N(1$^{\mathrm{I}}$)–N(1$^{\mathrm{II}}$)	3.44(2)	C(10$^{\mathrm{I}}$)–C(3$^{\mathrm{VI}}$)	3.73(2)
N(2$^{\mathrm{I}}$)–N(1$^{\mathrm{II}}$)	3.56(2)	C(11$^{\mathrm{I}}$)–C(4$^{\mathrm{VI}}$)	3.71(2)
N(2$^{\mathrm{I}}$)–O(1$^{\mathrm{II}}$)	3.69(2)	N(13$^{\mathrm{I}}$)–C(3$^{\mathrm{VI}}$)	3.74(2)
C(1$^{\mathrm{I}}$)–O(2$^{\mathrm{II}}$)	3.23(1)	C(5$^{\mathrm{I}}$)–C(11$^{\mathrm{IV}}$)	3.79(2)
C(1$^{\mathrm{I}}$)–N(1$^{\mathrm{II}}$)	3.68(2)	C(5$^{\mathrm{I}}$)–N(13$^{\mathrm{IV}}$)	3.43(2)
C(1$^{\mathrm{I}}$)–S$^{\mathrm{II}}$	3.75(1)	C(4$^{\mathrm{I}}$)–N(13$^{\mathrm{IV}}$)	3.59(2)
N(6$^{\mathrm{I}}$)–O(2$^{\mathrm{II}}$)	3.36(1)	C(5$^{\mathrm{II}}$)–N(13$^{\mathrm{VI}}$)	3.61(2)
O(1$^{\mathrm{I}}$)–C(9$^{\mathrm{VI}}$)	3.53(2)	C(4$^{\mathrm{II}}$)–C(4$^{\mathrm{VIII}}$)	3.65(2)
O(1$^{\mathrm{I}}$)–N(13$^{\mathrm{VI}}$)	3.72(2)	O(1$^{\mathrm{III}}$)–C(4$^{\mathrm{VI}}$)	3.33(2)

(b) Intramolecular bond distances (Å) and angles (deg.) for the sulphadiazine moiety

(i) Distances

N(1)–C(1)	1.42(2)	S–O(2)	1.48(1)
C(1)–N(2)	1.34(2)	S–C(7)	1.70(1)
N(2)–C(3)	1.34(2)	C(7)–C(8)	1.41(2)
C(3)–C(4)	1.38(2)	C(8)–C(0)	1.38(2)
C(4)–C(5)	1.33(2)	C(9)–C(10)	1.37(2)
C(5)–N(6)	1.33(2)	C(10)–N(13)	1.39(2)
N(6)–C(1)	1.31(3)	C(10)–C(11)	1.43(2)
S–N(1)	1.61(1)	C(11)–C(12)	1.44(2)
S–O(1)	1.45(1)	C(12)–C(7)	1.40(2)

(ii) Angles †

N(1)–S–O(2)	114	C(4)–C(5)–N(6)	123
O(2)–S–N(1)	115	C(5)–N(6)–C(1)	118
C(7)–S–N(1)	107	S–C(7)–C(8)	121
O(1)–S–C(7)	109	S–C(7)–C(12)	120
O(1)–S–N(1)	104	C(12)–C(7)–C(8)	118
O(2)–S–C(7)	107	C(7)–C(8)–C(9)	121
S–N(1)–C(1)	118	C(8)–C(9)–C(10)	123
N(1)–C(1)–N(6)	115	C(9)–C(10)–C(11)	118
N(1)–C(1)–N(2)	120	C(9)–C(10)–C(13)	122
N(6)–C(1)–N(2)	125	C(11)–C(10)–N(13)	118
C(1)–N(2)–C(3)	115	C(10)–C(11)–C(12)	119
N(2)–C(3)–C(4)	123	C(11)–C(12)–C(7)	121
C(3)–C(4)–C(5)	116		

* Roman numeral superscripts denote the following equivalent positions:

I x, y, z	V $x - 2, 1 - y, 1 - z$
II $1 - x, 1 - y, 1 - z$	VI $1 - x, y - \frac{1}{2}, \frac{1}{2} - z$
III $1 - x, \frac{1}{2} + y, \frac{1}{2} - z$	VII $1 + x, y, z$
IV $-x, \frac{1}{2} + y, \frac{1}{2} - z$	VIII $x, y - 1, z$

† Mean σ for all angles involving sulphur 1°; for other angles 1.5°.

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* See Notice to Authors No. 7 in *J.C.S. Perkin II*, 1974, Index issue.

with the (002) planes, and the benzene rings are close to the (020) planes.

Co-ordination of silver atoms occurs across the regions $c = 0$ and $c = \frac{1}{2}$ (Figure 2) to three separate sulphadiazine moieties. Each sulphadiazine molecule chelates one silver atom through O(2) and N(2), and bridges two others through N(1) and N(6). The bridged atoms are centrosymmetrically related (at $0,\frac{1}{2},\frac{1}{2}$). The configuration about each silver atom is approximately tetrahedral and the extent of the distortion is seen from the X–Ag–X angles [Table 2(*a*)]; Ag–N(1) and Ag–N(6) are the two strongest bonds (2.24 Å). These Ag–N distances are to be compared with those in a silver nitrate–pyrazine complex (2.21),[11] silver cyanate (2.11),[14] and in bis(imidazole)silver(I) nitrate (2.12 Å).[15,16] The silver atom is not co-ordinated to the amino-nitrogen atom [N(13)] as suggested by Fox,[7] and Sandmann's claim[6] that silver sulphadiazine forms a classical salt structure is incorrect.

TABLE 3

Bond distances (Å) and angles (deg.) in sulphonamides and related compounds, with estimated standard deviations in parentheses

Compound	S–O(1)	S–O(2)	S–N	S–C	N–C	O(1)–S–O(2)
Methane sulphonanilide [a]	1.452(2)	1.443(2)	1.633(2)	1.746(2)		118.6(1)
Sulphathiazole II [b]	1.444(2)	1.435(2)	1.588(3)	1.761(3)	1.401(4)	116.6(2)
β-Sulphanilamide [c]	1.44(1)	1.44(1)	1.63(1)	1.75(1)	1.38(2)	118.1(1)
β-Sulphanilamide [d]	1.454(2)	1.448(2)	1.620(2)	1.750(2)	1.385(6)	118.2(1)
α-Sulphanilamide [e]	1.47(2)	1.47(2)	1.61(2)	1.74(2)	1.40(2)	119(1)
Sulthiame [f]	1.47(1)	1.45(1)	1.63(1)	1.73(1)		115.9(5)
Sulthiame [f]	1.47(1)	1.46(1)	1.58(1)	1.76(1)		116.2(8)
γ-Sulphanilamide [g]	1.452(14)	1.438(19)	1.666(15)	1.739(14)	1.383(25)	117.3(9)
Sulphanilamide monohydrate [h]	1.463(9)	1.448(9)	1.620(11)	1.748(12)	1.377(16)	118.3(3)
Sulphamide [i]	1.39(1)		1.60(1)			119.4(8)
Silver sulphadiazine [j]	1.45(1)	1.48(2)	1.61(1)	1.70(1)	1.39(2)	114(1)

[a] Ref. 26. [b] Ref. 22. [c] Ref. 24. [d] Ref. 25. [e] Ref. 23. [f] Ref. 27. [g] M. Alléaume and J. Décap, *Acta Cryst.*, 1965, **19**, 934. [h] M. Alléaume and J. Décap, *Acta Cryst.*, 1968, **B24**, 214. [i] K. M. Trueblood and S. W. Mayer, *Acta Cryst.*, 1956, **9**, 628. [j] This work.

The Ag–O(2) distance (2.54 Å) corresponds to the upper limit of a normal weak covalent Ag–O bond and is similar to values reported for silver nitrate[19] and silver chlorite.[20] Much shorter Ag–O bond distances have been reported (2.11—2.19 Å)[15] and in a redetermination of the structure of silver nitrate, rather longer distances in the range 2.6—3.0 Å are also reported.[21]

The close silver–silver distance (2.916 Å) is comparable to that in the metal (2.889 Å). Similar close contacts have been reported in phenylethynyl(trimethylphosphine)silver(I) (3.03 Å),[13] and in (glycylglycine)silver(I) nitrate (2.92 Å).[14]

Although the nature of the analysis did not permit direct location of the hydrogen atoms, the interatomic vectors give strong evidence for hydrogen bonding. Infinite sheets of hydrogen bonds parallel to the (001) planes link the terminal NH_2 groups of the benzene rings to oxygen atoms of neighbouring molecules, each molecule being hydrogen bonded to four others. The N(13) atom forms two hydrogen bonds of medium strength to atoms O(1) and O(2) of separate molecules. The weak Ag–O(2) interaction does not appear significantly to alter the N(13)–O(2) bond length, although the S–O(2) bond length is lengthened relative to S–O(1), and to S–O bond lengths of related structures (see Table 3).[22-27] The hydrogen bonding system of silver sulphadiazine, despite the additional silver co-ordinations, is similar to those observed in related sulphonamide structures. It has been suggested[28] that strong hydrogen bonding contributes to the relative stability of polymorphs of sulphonamides, and polymorphism has been observed[29] in several sulphonamides but not in sulphadiazine. The present analysis has revealed a stable structure with pronounced hydrogen-bonding, low thermal parameters, but no evidence for polymorphism.

All the remaining short intermolecular distances (<3.8 Å) due to possible weak van der Waals interactions are given in Table 2(*a*). None appears to be of any great significance in the structure cohesion.

The Sulphadiazine Moiety.—The structure of the sulphadiazine moiety is given in Figure 3 and the intramolecular bond lengths and angles are listed in Table 2(*b*). The silver atom does not appreciably modify the sulphonamide structure and the dimensions are comparable to those of related structures.[22-27] Important bond distances and angles are given in Table 3 for these and other related compounds.

The stereochemistry about the sulphur atom is a slightly distorted tetrahedron, and the S–O(2) bond is longer than the S–O(1) bond due to the Ag–O(2) interaction (*vide supra*). The angle O(1)–S–O(2) is greater than the tetrahedral value but less than that found in the sulphonamides generally (Table 3). The S–N(1), S–C(2), and C(10)–N(13) bonds are much shorter than expected for pure single bonds and this is also observed in sulphonamides themselves, although the S–C bond is

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usually near 1.75 Å. This illustrates a partially quinoidal structure analogous to nitro-anilines,[25] and the intermediate bond character of the S–O(1), S–O(2), and S–N(1) bonds is maintained.[25]

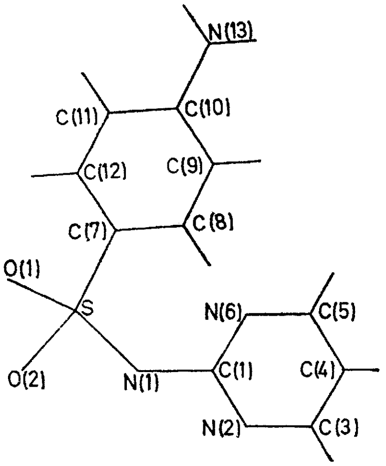

FIGURE 3 Sulphadiazine moiety of silver sulphadiazine

The dimensions of the pyrimidine ring are in general agreement with those for related heterocyclic structures,[30,31] although the N(1)–C(1) bond length is somewhat shorter than that reported for methane sulphonanilide (1.438 Å).[26]

Equations for least-squares planes for the benzene and pyrimidine rings together with their ring-attached atoms are given in Table 4. The pyrimidine ring is expectedly distorted from the planar configuration. The ring-attached sulphur atom is significantly displaced from the plane of the benzene ring, as has also been observed in α-sulphanilamide;[23] in β-sulphanilamide both the ring-attached sulphur and nitrogen atoms are displaced from the plane.[25] The dihedral angle between the planes of the two rings is 68°; 90° 44′ was reported[22] for sulphathiazole II.

TABLE 4

Least-squares planes equations in the form $lX + mY + nZ + P = 0$, where X, Y, and Z are orthogonal (Å) co-ordinates having X, Y, and Z along the a-, b-, and c^*-axes respectively. Deviations (Å) of atoms from the plane are given in square brackets

Plane (1): C(7)—(12), N(13), S

$$0.272X - 0.863Y - 0.426Z + 6.170 = 0$$

[C(7) 0.01, C(8) −0.03, C(9) 0.03, C(10) −0.01, C(11) 0, C(12) 0, N(13)* 0, S* −0.11]

Plane (2): C(1), N(2), C(3)—(5), N(6), N(1)

$$-0.254X - 0.029Y - 0.9672Z + 8.921 = 0$$

[C(1) 0.01, N(2) −0.03, C(3) 0.03, C(4) 0.01, C(5) −0.03, N(6) 0.02, N(1)* 0.01]

Dihedral angle (1)—(2) 68°

* Ring-attached atoms.

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