The structure of tris(phenylthio)amine (Carruthers, Prout & Watkin, 1981) differs markedly from that of tris(phenylthio)arsine: (1) N lies nearly in the plane of its three S atoms with an average S—N—S angle of 119·5°; (2) one of the N—S distances is significantly shorter (1·67 Å) than the other two (1·70, 1·71 Å); and (3) the phenyl rings are disposed such that the molecule deviates drastically from C_3 symmetry.

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Diamminebis(2-sulfanilamidopyrimidinato)zinc(II), $[Zn(C_{10}H_9N_4O_2S)_2(NH_3)_2]$

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Abstract. $M_r = 597·98$, orthorhombic, $Pn2_1a$, $a = 13·894\,(1)$, $b = 14·221\,(1)$, $c = 12·608\,(1)$ Å, $V = 2492·3$ Å^3, $Z = 4$, $D_x = 1·59$, $D_m = 1·59\,(1)$ g cm^{-3}, $\lambda(\text{Cu } K\alpha) = 1·54052$ Å, $\mu = 32·9$ cm^{-1}, $F(000) = 1232$, $T = 295$ K. Final $R_1 = 0·040$ for 3485 observed independent reflections. The Zn atom is surrounded by four N atoms: two from the ammonia molecules [2·036 (4) and 2·050 (4) Å] and two from the sulfanilamidopyrimidine ligands in a distorted tetrahedral arrangement. The two pyrimidine-containing ligands are coordinated at different sites: one ligand through the imido N atom [2·166 (4) Å] and one ligand through an N atom in the pyrimidine ring [2·078 (4) Å]. No significant differences in the pyrimidine rings are apparent, but the imido N—C and N—S distances are significantly longer for the imido N atom which is coordinated to the Zn atom.

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Introduction. The present structural investigation of the zinc sulfadiazine title complex was undertaken because of its effectiveness in preventing bacterial infection in burned animals (Fox, Modak & Stanford, 1978; Fox, Modak, Stanford & Fox, 1979). The related burn-treatment compound, (2-sulfanilamidopyrimidine)-silver(I), commercially used for burn treatment in patients as Silvadene, has a polymeric structure (Baenziger & Struss, 1976; Cook & Turner, 1975) which allows for the slow release of the Ag$^+$ ion, the active bactericidal ingredient (Fox & Modak, 1974; Modak & Fox, 1973) in the vicinity of the burn. The effectiveness of the burn-treatment compound does not appear to depend solely on the presence of Ag$^+$ (or Zn^{2+}) *per se*, but depends strongly on the nature of the material to which the metal ion is bound. The structure of the zinc sulfadiazine complex was undertaken to see if any common structural features exist between the silver and zinc complexes.

Experimental. Title compound synthesized as a fine powder from commercial sulfadiazine or sodium sulfadiazine plus a zinc salt [$Zn(NO_3)_2$ or $Zn(OAc)_2$] in aqueous solution. Single crystals of zinc sulfadiazine prepared by dissolving zinc sulfadiazine in ammonium hydroxide, driving off ammonia by heating the solution on a water bath until crystals began to appear, and continuing the crystallization in a refrigerator. Crystals analyzed for C, H and N gave: C 39·68, H 3·95, N 23·41%; theoretical for $C_{20}H_{24}N_{10}O_4S_2Zn$: C 40·37, H 4·03, N 23·34%; the complex is formulated as $[Zn(C_{10}H_9N_4O_2S)_2(NH_3)_2]$. D_m measured by flotation. Single-crystal intensity data (14376 reflections, $h \pm 15$, $k \pm 14$, $l \pm 15$) obtained with a FACS-I diffractometer, using a 2θ step-scan procedure (Baenziger, Foster, Howells, Howells, Vander Valk & Burton, 1977) (basic step size ranged from 0·08 to 0·15°); $2\theta_{\max} = 47°$. Averaging equivalent reflections ignoring non-equivalence of Friedel pairs yielded 2139 independent reflections of which 1941 had intensities greater than three standard deviations above background, average agreement among equivalent reflections 3%; averaging truly equivalent reflections gave 3645 reflections above $3\sigma_{\rm bkg}$, and an average among equivalent reflections of 2%. Data corrected for absorption; crystal bounding faces and distance between planes in mm: $\pm(010)$, 0·12; $\pm(111)$, 0·30; $\pm(\bar{1}12)$, 0·35; $\pm(\bar{2}10)$, 0·46; $\pm(0\bar{3}1)$, 0·25. Absorption correction 1·46–2·0 (Templeton & Templeton, 1973). Cell dimensions obtained from 12 reflections in angular range 100 to 120° 2θ. Three standard reflections 600, 060 and 006 varied in intensity by ±0·6, ±0·8 and ±1·0%, respectively. Structure solved by a combination of Patterson and *MULTAN* (Germain, Main & Woolfson, 1971) methods. Successive electron density maps eventually led to location of all heavy atoms, and 14 phenyl and pyrimidine H atoms located in a difference electron density map when $R = 0·09$; amine and ammonia H atoms located in a difference map when $R = 0·054$. In last refinement cycle, full-matrix least-squares program minimized $\sum w(\Delta F)^2$ for 333 parameters: anisotropic temperature factor parameters for all atoms except H. H atoms, though located in difference maps, were held at fixed positions and given an isotropic temperature factor equal to that of the atom to which they were attached plus ~0·5 Å^2. Atom scattering factors for Zn, S, O, N and C from *International Tables for X-ray Crystallography* (1974), for H from Stewart, Davidson & Simpson (1965); anomalous scattering corrections included for Zn and S. Weights used in refinement those estimated from counting statistics (S_{F^2}) corrected by an ignorance factor, $p = 0·07$, where weight $= 1/S^2$, $S = (S^2_{F^2} + p^2F_o{}^4)^{1/2}/2F_o$. With all atoms now included, R_1 became 0·044 based on 3551 present reflections. A number of low-angle reflections appeared to be subject to extinction effects; excluding those below $\sin\theta/\lambda = 0·15$ Å^{-1} left 3485 reflections, and final $R_1 = 0·040$, $R_2 = 0·059$. (Refinement of mirror-image structure yielded R_1 and R_2 values of 0·045 and 0·070; refinement of structure using averaged Friedel pairs gave R values of 0·045 and 0·056.) $(\Delta/\sigma)_{\max} = 0·07$. $\Delta\rho = -0·72$–$0·24$ e Å^{-3}. Computer programs used were local adaptations of Lawrence Radiation Laboratories, Berkeley, programs for least squares and electron density maps.

Discussion. Atomic positions are given in Table 1. Bond lengths and angles are given in Table 2.* The atom-numbering scheme is shown in Fig. 1.

The Zn atom is tetrahedrally (distorted) coordinated by two ammonia molecules and by N atoms from two sulfadiazine molecules. Different N atoms from the sulfadiazine molecule are involved in the coordination to the Zn atom. In the sulfadiazine molecule labeled *B*, the coordination is by the imido N atom, N(5*B*)

Table 1. *Atomic coordinates and equivalent isotropic thermal parameters for the non*-H *atoms*

$B_{\rm eq} = \frac{1}{3}(B_{11} + B_{22} + B_{33})$.

	x	y	z	$B_{\rm eq}$(Å^2)
Zn	0·25773 (4)	0	0·07747 (5)	4·23
S(2*A*)	0·40118 (7)	0·0756 (1)	0·34885 (8)	3·21
O(3*A*)	0·4770 (3)	0·1437 (2)	0·3285 (3)	3·9
O(4*A*)	0·3107 (3)	0·1164 (3)	0·3844 (3)	4·7
N(5*A*)	0·3754 (3)	0·0135 (3)	0·2501 (3)	3·3
C(6*A*)	0·4424 (3)	−0·0148 (3)	0·1794 (3)	2·8
N(7*A*)	0·4028 (3)	−0·0352 (2)	0·0837 (3)	2·7
C(8*A*)	0·4620 (3)	−0·0647 (3)	0·0068 (4)	3·5
C(9*A*)	0·5591 (3)	−0·0716 (3)	0·0212 (3)	3·5
C(10*A*)	0·5929 (3)	−0·0505 (3)	0·1203 (4)	3·3
N(11*A*)	0·5357 (3)	−0·0229 (3)	0·2012 (3)	3·3
C(12*A*)	0·4429 (3)	0·0034 (4)	0·4527 (3)	3·3
C(13*A*)	0·4904 (3)	0·0456 (3)	0·5364 (4)	3·6
C(14*A*)	0·5145 (3)	−0·0073 (4)	0·6243 (4)	3·9
C(15*A*)	0·4941 (3)	−0·1030 (3)	0·6286 (4)	3·4
C(16*A*)	0·4478 (3)	−0·1445 (3)	0·5420 (4)	3·8
C(17*A*)	0·4217 (3)	−0·0911 (3)	0·4550 (4)	3·6
N(18*A*)	0·5125 (3)	−0·1546 (4)	0·7202 (4)	4·6
S(2*B*)	0·30011 (7)	0·19850 (9)	−0·07394 (7)	2·76
O(3*B*)	0·2661 (2)	0·2426 (3)	−0·1700 (3)	3·5
O(4*B*)	0·2745 (2)	0·2442 (3)	0·0248 (3)	3·8
N(5*B*)	0·2647 (3)	0·0916 (3)	−0·0596 (3)	3·0
C(6*B*)	0·2648 (3)	0·0269 (3)	−0·1403 (3)	2·8
N(7*B*)	0·2488 (3)	−0·0608 (3)	−0·1004 (3)	3·3
C(8*B*)	0·2451 (3)	−0·1315 (4)	−0·1695 (5)	4·0
C(9*B*)	0·2563 (3)	−0·1167 (4)	−0·2764 (5)	4·0
C(10*B*)	0·2754 (4)	−0·0264 (4)	−0·3083 (4)	3·8
N(11*B*)	0·2795 (3)	0·0473 (3)	−0·2427 (3)	3·0
C(12*B*)	0·4268 (3)	0·1944 (3)	−0·0788 (3)	2·4
C(13*B*)	0·4730 (3)	0·2000 (4)	−0·1750 (3)	3·3
C(14*B*)	0·5747 (3)	0·1978 (4)	−0·1770 (3)	3·5
C(15*B*)	0·6269 (3)	0·1897 (3)	−0·0825 (3)	2·9
C(16*B*)	0·5774 (3)	0·1846 (3)	0·0135 (3)	3·1
C(17*B*)	0·4780 (3)	0·1878 (3)	0·0148 (3)	2·8
N(18*B*)	0·7264 (3)	0·1896 (3)	−0·0850 (3)	3·5
N(19)	0·1779 (3)	−0·1129 (3)	0·1235 (4)	4·8
N(20)	0·1914 (3)	0·0996 (3)	0·1696 (3)	3·8

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* Lists of structure factors, anisotropic thermal parameters, H-atom positions, least-squares-planes' data and interatomic distances and angles for the phenyl groups and bonds involving H have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 38699 (21 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

(2·166 Å). In molecule *A*, one of the pyrimidine ring N atoms, N(7*A*) (2·078 Å), is coordinated. The atoms N(5*A*) and N(7*B*) are located much farther away (2·729 and 2·406 Å).

With coordination at different N atoms in the two ligands, it might be expected that the two ligands would differ in their internal bonding arrangement, and that these differences would be greatest in the pyrimidine part of the ligand. However, the two ligands are nearly identical, significant differences being present only in the sulfonamido group. The two phenyl groups are essentially the same in the two molecules: the average

Table 2. *Interatomic distances* (Å) *and bond angles* (°) *in* [Zn(*SD*)$_2$(NH$_3$)$_2$] *and comparisons to related structures* [*SD*=2-*sulfanilamidopyrimidine* (*sulfadiazine*)]

Zn—N(19)	2·036 (4)
Zn—N(20)	2·050 (4)

	Ligand *A*	Ligand *B*	SD (*a*)	SD (*b*)	5-Methoxy SD (*c*) Form (I)	5-Methoxy SD (*c*) Form (I′)	5-Methoxy SD (*c*) Form (III)
Zn—N(5)	2·729 (4)	2·166 (4)					
Zn—N(7)	2·078 (4)	2·406 (4)					
S(2)—N(5)	1·568 (4)	1·609 (4)	1·660	1·654 (2)	1·644	1·657	1·645
S(2)—C(12)	1·762 (5)	1·762 (4)	1·740	1·745 (3)	1·737	1·739	1·741
S(2)—O(3)	1·453 (4)	1·443 (4)	1·410	1·423 (2)	1·434	1·431	1·429
S(2)—O(4)	1·455 (3)	1·449 (3)	1·420	1·430 (2)	1·449	1·442	1·451
N(5)—C(6)	1·350 (5)	1·372 (6)	1·380	1·375 (3)	1·401	1·421	1·398
C(6)—N(11)	1·330 (5)	1·338 (6)	1·310	1·325 (4)	1·316	1·313	1·317
C(6)—N(7)	1·357 (5)	1·363 (6)	1·310	1·334 (4)	1·330	1·340	1·336
N(11)—C(10)	1·351 (6)	1·336 (6)	1·330	1·338 (4)	1·351	1·328	1·347
N(7)—C(8)	1·339 (6)	1·332 (7)	1·370	1·337 (3)	1·336	1·342	1·333
C(8)—C(9)	1·365 (7)	1·372 (9)	1·360	1·374 (4)	1·379	1·377	1·381
C(9)—C(10)	1·368 (7)	1·372 (8)	1·380	1·374 (4)	1·377	1·390	1·380
Phenyl C—C av.	1·385	1·391					
E.s.d. in C—C distance	0·007	0·006					
Scatter in C—C distance	0·007	0·015					
C—N(NH$_2$)	1·391 (7)	1·382 (6)					

Selected next nearest neighbor distances–comparing the conformations of ligand *A* and *B*

	Ligand *A*	Ligand *B*		Ligand *A*	Ligand *B*		Ligand *A*	Ligand *B*		Ligand *A*	Ligand *B*
S(2)—C(13)	2·704 (5)	2·719 (5)	N(5)—O(3)	2·529 (5)	2·559 (6)	O(3)—N(11)	2·976 (5)	2·931 (5)	O(3)—C(13)	2·974 (7)	2·938 (6)
S(2)—C(12)	2·737 (5)	2·717 (4)	N(5)—O(4)	2·413 (5)	2·421 (5)	O(3)—C(6)	2·974 (5)	3·090 (6)	O(4)—N(5)	2·413 (5)	2·421 (5)
S(2)—C(16)	2·559 (4)	2·627 (4)	N(5)—O(7)	2·241 (5)	2·238 (6)	O(3)—N(5)	2·529 (5)	2·559 (6)	O(4)—C(12)	2·587 (6)	2·585 (5)
S(2)—N(11)	2·987 (4)	3·039 (4)	N(5)—N(11)	2·368 (5)	2·402 (5)	O(3)—C(12)	2·580 (6)	2·603 (5)	O(4)—C(17)	3·304 (6)	2·942 (6)

N(5*B*)—Zn—N(7*A*)	97·6 (2)	N(5*B*)—Zn—N(20)	93·2 (2)	N(7*A*)—Zn—N(20)	125·5 (2)
N(5*B*)—Zn—N(19)	136·5 (2)	N(7*A*)—Zn—N(19)	109·1 (2)	N(19)—Zn—N(20)	98·0 (2)

	Ligand *A*	Ligand *B*		Ligand *A*	Ligand *B*		Ligand *A*	Ligand *B*
O(3)—S(2)—O(4)	114·5 (3)	116·5 (3)	S(2)—N(5)—Zn	144·0 (3)	132·1 (3)	C(6)—N(7)—Zn	112·1 (4)	90·0 (4)
O(3)—S(2)—N(5)	113·6 (3)	113·9 (3)	C(6)—N(5)—Zn	82·3 (3)	100·9 (3)	Zn—N(7)—C(8)	130·1 (4)	152·1 (4)
O(3)—S(2)—C(12)	106·3 (3)	108·2 (3)	N(5)—C(6)—N(7)	111·8 (3)	109·8 (4)	N(7)—C(8)—C(9)	122·2 (4)	121·5 (4)
O(4)—S(2)—N(5)	105·8 (3)	104·6 (3)	N(5)—C(6)—N(11)	124·1 (4)	124·8 (4)	C(8)—C(9)—C(10)	116·0 (4)	117·0 (5)
O(4)—S(2)—C(12)	106·7 (3)	106·8 (3)	N(7)—C(6)—N(11)	124·1 (4)	125·4 (4)	C(9)—C(10)—N(11)	123·4 (4)	124·1 (4)
N(5)—S(2)—C(12)	109·7 (3)	106·2 (3)	C(6)—N(7)—C(8)	117·5 (4)	117·1 (4)	C(10)—N(11)—C(6)	116·3 (4)	114·9 (4)
S(2)—N(5)—C(6)	122·4 (3)	123·4 (3)						
Av. C—C—C angle in phenyl rings	120·0	120·0						
E.s.d. in angle	0·4	0·4						
Scatter in angle	1·0	0·9						
C(14)—C(15)—N(18)	120·7 (4)	119·8 (4)						
N(18)—C(15)—C(16)	120·7 (4)	120·9 (4)						

Distances (Å) and angles (°) relevant to hydrogen bonds

N(18*A*)—O(3*A*$^{\rm ii}$)	2·938 (6)	H(182*A*)—O(3*A*$^{\rm ii}$)	2·031	C(15*A*)—N(18*A*)···O(3*A*$^{\rm ii}$)	110·5 (5)
N(18*B*)—O(4*A*$^{\rm i}$)	2·976 (5)	H(182*B*)—O(4*A*$^{\rm i}$)	2·074	C(15*B*)—N(18*B*)···O(4*A*$^{\rm i}$)	107·7 (5)
N(18*B*)—N(11*A*$^{\rm i}$)	3·060 (6)	H(181*B*)—N(118$^{\rm i}$)	2·151	C(15*B*)—N(18*B*)···N(11*B*$^{\rm i}$)	104·9 (5)
N(18*B*)—N(19$^{\rm ii}$)	3·145 (7)				
N(18*B*)—O(3*B*$^{\rm i}$)	3·227 (6)				
N(19)—N(20)	3·083 (6)				
N(19)—N(7*B*)	3·080 (6)				
N(19)—N(18*B*$^{\rm ii}$)	3·144 (2)	H(193)—H(18*B*$^{\rm ii}$)	2·433	Zn—N(19)—N(18*B*$^{\rm ii}$)	115·5 (4)
N(19)—N(11*A*$^{\rm i}$)	3·220 (5)	H(192)—N(11*A*$^{\rm i}$)	2·548	Zn—N(19)—N(11*A*$^{\rm i}$)	102·4 (4)
N(19)—N(7*A*)	3·352 (6)				
N(19)—O(3*B*$^{\rm iii}$)	3·407 (7)	H(193)—O(3*B*$^{\rm iii}$)	2·564	Zn—N(19)—O(3*B*$^{\rm iii}$)	124·7 (4)
N(20)—O(4*B*)	2·982 (6)	H(203)—O(4*B*)	2·070	Zn—N(20)—O(4*B*)	87·5 (4)
N(20)—N(5*A*)	3·012 (5)				
N(20)—O(3*A*$^{\rm i}$)	3·044 (6)	H(201)—O(3*A*$^{\rm i}$)	2·205	Zn—N(20)—O(3*A*$^{\rm i}$)	125·9 (4)
N(20)—N(5*B*)	3·065 (6)				
N(20)—O(4*A*)	3·186 (6)	H(202)—O(4*A*)	2·389	Zn—N(20)—O(4*A*)	107·4 (4)
N(20)—N(11*A*$^{\rm i}$)	3·220 (5)				

Symmetry translations: (i) $\frac{1}{2}+x, y, \frac{1}{2}-z$; (ii) $-x, \frac{1}{2}+y, -z$; (iii) $\frac{1}{2}-x, \frac{1}{2}+y, \frac{1}{2}+z$.

Notes: (*a*) Shin, Ihn, Kim & Koo (1974). (*b*) Unpublished work by authors [C—C error 0·003 to 0·004 Å; S—(C,O,N) error 0·002 Å]. (*c*) Giuseppetti, Tadini, Bettinetti & Giordano (1977).

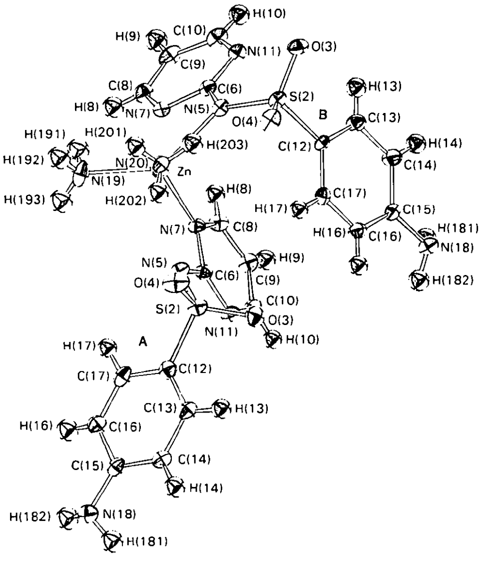

Fig. 1. Perspective view of a molecule of the title compound.

C—C distance is 1·385 Å, scatter ±0·007 Å in *A*; 1·391 Å, scatter ±0·015 Å in *B*; individual atom-position errors are ±0·006 to 0·007 Å.

The biggest differences in bond distances between ligand *A* and ligand *B* occur in the N(5)—S(2) bond distance, 0·041 Å longer in ligand *B* which is complexed to Zn at N(5); in N(5)—C(6), which is 0·022 Å longer in ligand *B*; and in N(11)—C(10), which is 0·16 Å longer in ligand *A* where the pyrimidine ring is complexed at N(7). It also should be pointed out that it is the N(5)—C(6) distance in the complexes which shows the greatest change from the bond distances observed in the uncomplexed pyrimidine structures already reported. The N(5)—C(6) bond distance is significantly shorter in the complexed ligand *A*. The S(2)—C(12) distances are significantly longer in the complexes as compared to the uncomplexed ligands, and the C(6)—N(7) and C(6)—N(11) pyrimidine bond distances also appear to be lengthened in the complexes.

The rather small differences in bond distances observed between ligands *A* and *B* may be due, in part, to the fact that although they might be characterized as ligand *A* coordinated at a pyrimidine N atom and ligand *B* coordinated at the imido N atom, the pyrimidine N(7) in ligand *B* is also 2·406 Å from the Zn atom and may also be involved in the coordination. [The imido N(5) atom in ligand *A* at 2·729 Å from the Zn atom is probably too far away to be involved significantly in bonding. It is interesting to note, however, that the combination of the distances 2·078 and 2·729 Å in ligand *A* and 2·166 and 2·406 Å in ligand *B* each combine to produce almost the same total bonding as judged from Pauling's (1947) bond order–bond-length relationship as the Zn atom bonds to the NH_3 groups.]

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Dichloro[(4*S*,7*R*)-7,8,8-trimethyl-2-(2-pyridyl)-4,5,6,7-tetrahydro-4,7-methano-2*H*-indazole]palladium(II), $C_{16}H_{19}Cl_2N_3Pd$

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Abstract. $M_r = 430{\cdot}66$, orthorhombic, $P2_12_12_1$, $a = 13{\cdot}154\ (2)$, $b = 15{\cdot}394\ (4)$, $c = 8{\cdot}402\ (2)$ Å, $V = 1701{\cdot}4$ Å^3, $Z = 4$, $D_m = 1{\cdot}66\ (1)$, $D_x = 1{\cdot}68$ g cm^{-3}, $\lambda(\text{Mo } K\alpha) = 0{\cdot}71069$ Å, $\mu = 13{\cdot}8$ cm^{-1}, $F(000) = 864$, $T = 293$ K. Final $R = 0{\cdot}035$ for 1659 observed reflections. The pyrazole and pyridine rings are both planar

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