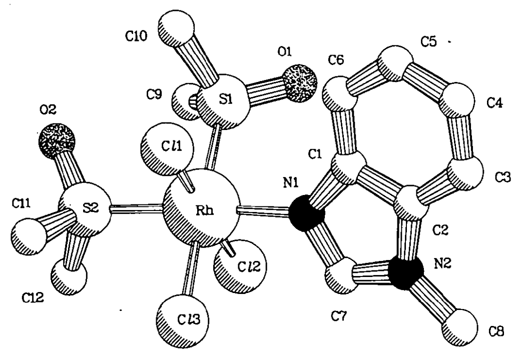

Fig. 1. *PLUTO* (*EUCLID* version) drawing of the title compound with the adopted atom numbering. Hydrogen atoms and the Me$_2$SO molecule of crystallization are omitted for clarity.

molecules of crystallization. The Rh atom is octahedrally coordinated by two S atoms of Me$_2$SO molecules, three Cl atoms and an N atom of the 1-methylbenzimidazole ligand. The small deviation from octahedral coordination is illustrated by the range [86·91 (6)–93·43 (6)°] of the 12 angles with ideal values of 90°. The Rh—Cl distances of 2·340 (2), 2·341 (2) and 2·358 (2) Å for Cl(1), Cl(2) and Cl(3) respectively are similar to the corresponding Rh—Cl distances in the related trichloro(dimethylformamide)-bis(dimethyl sulfoxide)rhodium(III) complex which are 2·329 (1), 2·343 (1) and 2·366 (1) Å (Rochon, Kong & Melanson, 1983). In the present structure the Rh—Cl(3) bond, being in *trans* position with respect to an Me$_2$SO molecule, is significantly (6σ) longer than the two other mutually *trans*-positioned Rh—Cl bonds; this effect was also found by Rochon *et al.* (1983). The range of the six Rh—Cl distances found in trichloro(dimethyl sulfoxide)bispyridinerhodium(III) (Colamarino & Orioli, 1976) is 2·314 (5)–2·348 (4) Å. The Rh—S distances in the title compound are 2·290 (2) and 2·286 (2) Å for S(1) and S(2) respectively; they compare well with the values found in the Rh–pyridine complex: 2·284 (5) and 2·283 (4) Å. The Rh—S distances found in the Rh–dimethylformamide complex are 2·290 (1) and 2·242 (1) Å. The present Rh—N(1) distance of 2·098 (5) Å is different from the average Rh—N distance [2·05 (1) Å] found in the Rh–pyridine complex. This might be caused by the different nature of the pyridine and benzimidazole ligands.

The geometry of the benzimidazole moiety compares well with the geometry of a similar fragment also bonded with an N atom to a transition metal in dichlorobis[1-(2-pyridylmethyl)benzimidazole]cobalt (Sundberg, Yilmaz & Mente, 1977). The largest differences between corresponding bond distances and angles are 0·018 Å and 2·0° respectively.

The X-ray data were collected by A. J. M. Duisenberg. The investigation was supported in part (WJJS and ALS) by the Netherlands Foundation for Chemical Research (SON) with financial aid from the Netherlands Organization for Advancement of Pure Research (ZWO).

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Diamminebis[*N'*-(2-pyrimidinyl)sulfanilamido]copper*

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Abstract. [Cu(C$_{10}$H$_9$N$_4$O$_2$S)$_2$(NH$_3$)$_2$], $M_r = 596·15$, orthorhombic, $Pn2_1a$ (equivalent positions x,y,z; $\frac{1}{2}-x$, $\frac{1}{2}+y$, $\frac{1}{2}+z$; $-x$, $\frac{1}{2}+y$, $-z$; $\frac{1}{2}+x$, y, $\frac{1}{2}-z$), $a = 13·915$ (5), $b = 14·356$ (5), $c = 12·659$ (5) Å, $V = 2528·81$ Å^3, $Z = 4$, $D_m = 1·55$ (1), $D_x = 1·566$ Mg m^{-3}, λ(Mo $K\alpha$) $= 0·71069$ Å, $\mu = 1·11$ mm^{-1}, $F(000) = 1228$, $T =$

* Copper sulphadiazine diammoniate.

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Table 1. *Final atomic parameters and e.s.d.'s*

$$B_{eq} = \tfrac{4}{3}(\beta_{11}/a^{*2} + \beta_{22}/b^{*2} + \beta_{33}/c^{*2}).$$

	x	y	z	B_{eq}(Å^2)
Cu	0·24663 (8)	0·29738	0·93651 (10)	3·03 (2)
S(1)	0·3010 (2)	0·0955 (3)	1·0716 (2)	2·11 (3)
S(2)	0·4035 (2)	0·2162 (3)	0·6557 (2)	2·40 (3)
O(1)	0·2627 (4)	0·0466 (7)	1·1624 (6)	2·72 (11)
O(2)	0·2700 (7)	0·0470 (9)	0·9772 (9)	4·87 (17)
O(3)	0·4857 (6)	0·1567 (8)	0·6715 (6)	3·78 (13)
O(4)	0·3123 (7)	0·1757 (10)	0·6282 (9)	5·54 (19)
N(1)	0·2688 (7)	0·2062 (12)	1·0610 (7)	4·10 (16)
N(2)	0·7255 (9)	0·1187 (14)	1·0854 (10)	3·90 (19)
N(3)	0·2544 (9)	0·3631 (13)	1·1174 (14)	5·72 (29)
N(4)	0·2911 (6)	0·2568 (7)	1·2394 (6)	2·44 (12)
N(5)	0·3658 (7)	0·2840 (9)	0·7556 (9)	4·78 (16)
N(6)	0·5098 (12)	0·4348 (13)	0·2778 (14)	6·73 (33)
N(7)	0·5280 (7)	0·3230 (8)	0·8143 (7)	3·05 (15)
N(8)	0·4155 (7)	0·3219 (8)	0·9327 (6)	3·82 (16)
N(9)	0·1933 (5)	0·1883 (8)	0·8452 (7)	3·08 (13)
N(10)	0·1839 (6)	0·3888 (8)	0·8536 (7)	2·99 (13)
C(1)	0·4274 (10)	0·1002 (14)	1·0730 (10)	4·48 (22)
C(2)	0·4814 (11)	0·1050 (19)	0·9818 (14)	5·24 (29)
C(3)	0·5813 (9)	0·1111 (10)	0·9841 (8)	4·21 (18)
C(4)	0·6271 (8)	0·1129 (10)	1·0810 (10)	3·61 (18)
C(5)	0·5759 (15)	0·1079 (18)	1·1742 (14)	5·21 (31)
C(6)	0·4757 (10)	0·1021 (12)	1·1682 (11)	5·04 (25)
C(7)	0·2712 (9)	0·2742 (12)	1·1378 (10)	2·76 (19)
C(8)	0·2546 (8)	0·4376 (14)	1·1822 (11)	3·68 (23)
C(9)	0·2754 (18)	0·4180 (17)	1·2865 (14)	5·64 (35)
C(10)	0·2933 (9)	0·3251 (13)	1·3142 (9)	3·20 (20)
C(11)	0·4486 (11)	0·2846 (15)	0·5526 (11)	5·85 (29)
C(12)	0·4227 (8)	0·3780 (10)	0·5428 (10)	3·46 (19)
C(13)	0·4432 (12)	0·4285 (13)	0·4521 (11)	4·45 (26)
C(14)	0·4901 (14)	0·3849 (17)	0·3677 (15)	5·61 (34)
C(15)	0·5154 (10)	0·2929 (14)	0·3774 (12)	4·58 (24)
C(16)	0·4948 (12)	0·2413 (16)	0·4682 (12)	6·34 (30)
C(17)	0·4344 (16)	0·3081 (17)	0·8302 (15)	6·36 (34)
C(18)	0·5996 (10)	0·3466 (13)	0·8781 (10)	4·34 (25)
C(19)	0·5736 (9)	0·3579 (11)	0·9824 (9)	3·91 (18)
C(20)	0·4773 (8)	0·3455 (12)	1·0104 (9)	3·47 (19)

295 K, $R = 0·045$ for 1417 observed diffractometer reflexions $[I/\sigma(I) \geq 1]$. The Cu atom coordinates to five N atoms in a distorted square-pyramidal arrangement. The basal plane contains two N atoms from one sulfadiazine and two from ammonia molecules. One N from the second sulfadiazine occupies the apex. The two rings of each sulfadiazine molecule are inclined to each other by + 94·17 (5) and + 91·76 (5)°, and are linked to each other and to the ammonia molecules by a three-dimensional hydrogen-bond system with lengths between 2·837 and 3·251 (16) Å. Bond lengths and inter-bond angles are normal.

Introduction. Sulfadiazine compounds are widely used pharmacologically for their bactericidal action and the metal complexes promote rapid healing of skin disorders (*e.g.* 'Flammazine', marketed by Smith & Nephew Ltd). The crystal structures of silver sulfadiazine (Cook & Turner, 1975) and zinc sulfadiazine (Brown, Cook & Sengier, 1985) have already been reported, and this investigation was undertaken because the Cu and Zn complexes had similar unit-cell dimensions and the same space group; it was therefore of interest to compare the coordinations of the metal atoms in the two structures.

Experimental. Samples supplied by Smith & Nephew Ltd, Harlow, Essex; m.p. 507 K(dec.); analysis gave

Table 2. *Bond lengths* (Å) *and inter-bond angles* (°)

Cu—N(1)	2·071 (13)	N(3)—C(7)	1·323 (25)
Cu—N(3)	2·479 (18)	N(3)—C(8)	1·348 (26)
Cu—N(8)	2·377 (10)	N(4)—C(7)	1·340 (15)
Cu—N(9)	2·083 (11)	N(4)—C(10)	1·362 (18)
Cu—N(10)	1·894 (10)	N(5)—C(17)	1·387 (24)
S(1)—O(1)	1·449 (8)	N(6)—C(14)	1·373 (27)
S(1)—O(2)	1·448 (12)	N(7)—C(17)	1·336 (24)
S(1)—N(1)	1·657 (17)	N(7)—C(18)	1·327 (17)
S(1)—C(1)	1·760 (14)	N(8)—C(17)	1·338 (21)
S(2)—O(3)	1·442 (10)	N(8)—C(20)	1·350 (15)
S(2)—O(4)	1·439 (11)	C—C(phenyl)$_{mean}$	1·388 (22)
S(2)—N(5)	1·680 (12)	C(8)—C(9)	1·381 (24)
S(2)—C(11)	1·750 (17)	C(9)—C(10)	1·401 (30)
N(1)—C(7)	1·378 (20)	C(18)—C(19)	1·379 (18)
N(2)—C(4)	1·372 (17)	C(19)—C(20)	1·397 (16)

N(1)—Cu—N(3)	62·0 (5)	S(2)—N(5)—C(17)	116·2 (1·2)
N(1)—Cu—N(8)	87·8 (4)	C(17)—N(7)—C(18)	132·9 (1·4)
N(1)—Cu—N(9)	90·0 (4)	C(17)—N(8)—C(20)	128·2 (1·3)
N(1)—Cu—N(10)	158·2 (5)	C—C—C(phenyl)$_{mean}$	120·0 (1·5)
N(3)—Cu—N(8)	85·4 (5)	S(1)—C(1)—C(2)	122·6 (1·3)
N(3)—Cu—N(9)	144·5 (5)	S(1)—C(1)—C(6)	119·8 (1·2)
N(3)—Cu—N(10)	105·6 (5)	N(2)—C(4)—C(3)	119·8 (1·2)
N(8)—Cu—N(9)	116·9 (4)	N(2)—C(4)—C(5)	118·9 (1·4)
N(8)—Cu—N(10)	110·0 (4)	N(1)—C(7)—N(3)	122·8 (1·4)
N(9)—Cu—N(10)	92·8 (4)	N(1)—C(7)—N(4)	123·4 (1·2)
O(1)—S(1)—O(2)	108·2 (6)	N(3)—C(7)—N(4)	113·8 (1·3)
O(1)—S(1)—N(1)	115·4 (6)	N(3)—C(8)—C(9)	114·8 (1·6)
O(1)—S(1)—C(1)	112·2 (6)	C(8)—C(9)—C(10)	118·1 (1·8)
O(2)—S(1)—N(1)	108·3 (7)	N(4)—C(10)—C9)	120·5 (1·4)
O(2)—S(1)—C(1)	108·9 (7)	S(2)—C(11)—C(12)	120·9 (1·3)
N(1)—S(1)—C(1)	103·5 (7)	S(2)—C(11)—C(16)	119·1 (1·4)
O(3)—S(2)—O(4)	119·6 (6)	N(6)—C(14)—C(13)	119·6 (1·8)
O(3)—S(2)—N(5)	119·2 (6)	N(6)—C(14)—C(15)	121·6 (1·8)
O(3)—S(2)—C(11)	98·7 (7)	N(5)—C(17)—N(7)	127·5 (1·8)
O(4)—S(2)—N(5)	98·1 (6)	N(5)—C(17)—N(8)	124·2 (1·8)
O(4)—S(2)—C(11)	111·3 (8)	N(7)—C(17)—N(8)	108·3 (1·6)
N(5)—S(2)—C(11)	110·4 (7)	N(7)—C(18)—C(19)	114·6 (1·3)
S(1)—N(1)—C(7)	128·0 (1·0)	C(18)—C(19)—C(20)	118·7 (1·3)
C(7)—N(3)—C(8)	130·3 (1·6)	N(8)—C(20)—C(19)	117·2 (1·2)
C(7)—N(4)—C(10)	122·6 (1·1)		

Cu 10·95, C 39·65, H 4·07, N 23·83% (required for $C_{20}H_{24}CuN_{10}O_4S_2$: Cu 10·66, C 40·30, H 4·06, N 23·50%). Dark green needle-shaped crystals $\simeq 0·05 \times 0·05 \times 1·0$ mm from 10% ammonia solution in the dark. D_m by flotation in NaI solution. Lattice parameters initially from Stoe Reciprocal Lattice Explorer, subsequently refined by least-squares methods based on 16 setting angles ($6 \leq 2\theta \leq 48°$) measured on the diffractometer. Intensities measured on Stoe Stadi-2 diffractometer using graphite-monochromatized Mo $K\alpha$ radiation; $2\theta_{max} = 50°$, index range h 0→16, k 0→9, l 0→15; ten standard reflexions, no variation; 1681 measured reflexions, of which 264 had $I < 1\sigma(I)$; corrections for Lp but not for absorption or extinction; Patterson synthesis showed structural similarity to Zn complex so coordinates of that used as starting point for structure determination; refinement by least squares on F using *NRC* programs (Ahmed, Hall, Pippy & Huber, 1970) on a VAX 11/750 computer; H atoms by calculation and used in F calculations with $B_{iso} = 7·0$ Å^2 but not refined; non-H atoms refined anisotropically until $\Delta/\sigma(\max) < 0·5$; residual $\Delta\rho$ in final difference map within $\pm 0·25$ e Å^{-3}; scattering factors from *International*

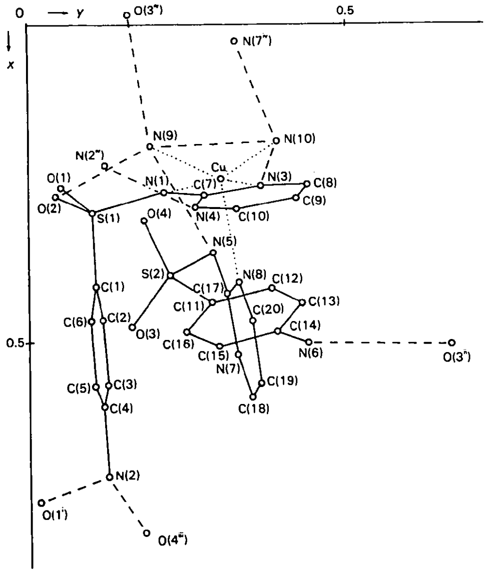

Fig. 1. Arrangement of molecule in (001) projection of part of unit-cell contents, showing atom numbering, copper coordination (dotted lines) and H-bonding system (dashed lines). Symmetry code: (i) $\frac{1}{2}+x, y, \frac{1}{2}-z$; (ii) $1-x, \frac{1}{2}+y, 1-z$; (iii) $\frac{1}{2}+x, y, 1\frac{1}{2}-z$; (iv) $x-\frac{1}{2}, y, 1\frac{1}{2}-z$; (v) $1-x, \frac{1}{2}+y, -z$.

Tables for X-ray Crystallography (1974); $R = 0.045$, $wR = 0.080$, $w^{1/2} = 1/F_o$.

Discussion. Atomic coordinates and equivalent isotropic temperature factors are listed in Table 1,* and selected bond lengths and interbond angles are listed in Table 2.

* Lists of structure factors, anisotropic thermal parameters, H-atom parameters, phenyl-ring bonds and angles, mean planes and H bonds have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44303 (15 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

The Cu atom is 5-coordinated in a distorted square pyramid, with N(1), N(3), N(9) and N(10) at distances 2·071 (13), 2·479 (18), 2·083 (11) and 1·894 (10) Å, respectively, in an irregular square, with a mean N—Cu—N angle, subtended by adjacent N atoms, of 87·6 (4)°. Atom N(8) at 2·377 (10) Å is at the apex with a mean N(8)—Cu—N angle of 100·0 (4)°. This 5-coordination in the Cu complex compares with the nearly regular tetrahedral coordination in the Zn complex (Brown, Cook & Sengier, 1985) where only N(1), N(8), N(9) and N(10) are used, N(3) being outside the sphere of coordination.

The intramolecular bond lengths and angles all agree well with the values found in this class of compound as well as in sulfamethazine (Basak, Mazumdar & Chaudhuri, 1983). The four organic molecular rings are each effectively planar with r.m.s. deviations all < 0·006 Å. The dihedral angles between the phenyl and diazine rings of each molecule are +94·17 (5) and +91·76 (5)°. There are eight probable hydrogen bonds of lengths between 2·837 (16) and 3·251 (21) Å, but as the electron density on difference maps around the N atoms was somewhat diffuse there is no certainty about these. The likely H-bond arrangement (Fig. 1) shows some differences from that in the Zn complex, and this may give rise to the differences in the unit-cell dimensions.

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Structure of Dichloro(4,7-diphenyl-1,10-phenanthroline)palladium(II)

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Abstract. $[PdCl_2(C_{24}H_{16}N_2)]$, $M_r = 509·4$, monoclinic, $P2_1/n$, $a = 15·354$ (2), $b = 17·551$ (3), $c = 15·665$ (1) Å, $\beta = 105·33$ (1)°, $V = 4071$ Å^3, $Z = 8$, $D_x = 1·66$ g cm^{-3}, λ(Mo $K\alpha$) = 0·71069 Å, $\mu = 11·73$ cm^{-1}, $F(000) = 2032$, $T = 293$ K, final $R = 0·035$ for 6324 observed reflections [$I > 2\sigma(I)$]. In both independent molecules a planar, bidentate 1,10-phenanthroline ligand is chelated to a $PdCl_2$ entity. The

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