rings are planar within 0·005 Å with interplanar angles between the free rings of 75·2(2)° [78·4(2)°] and between the free and the anchored rings of 74·4 (2)° [73·5 (2)°] and 85·4 (2)° [82·2 (2)°].

The shortest intermolecular contacts are between H···H (2·36 Å) C···H (2·74 Å) and Cl···H (2·75 Å).

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Structure of Trichlorobis(dimethyl sulfoxide)(1-methylbenzimidazole)rhodium(III) Dimethyl Sulfoxide Solvate

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Abstract. $[RhCl_3(C_2H_6OS)_2(C_8H_8N_2)].C_2H_6OS$, M_r = 575·82, orthorhombic, *Pbca*, a = 14·088 (3), b = 15·774 (8), c = 20·623 (5) Å, V = 4583 (3) Å^3, Z = 8, D_x = 1·669 g cm^{-3}, λ(Mo $K\alpha$) = 0·71073 Å, μ = 13·7 cm^{-1}, $F(000)$ = 2336, T = 295 K, R = 0·0440 for 2554 observed reflections with $I > 2\sigma(I)$. The Rh atom is octahedrally coordinated by three meridional Cl atoms, two *cis* sulfur-bonded dimethyl sulfoxide molecules and an N atom of the 1-methylbenzimidazole ligand. The Rh—Cl bond [2·358 (2) Å] *trans* to dimethyl sulfoxide is significantly longer than the two mutually *trans*-positioned Rh—Cl bonds [2·340 (2), 2·341 (2) Å].

Introduction. In the course of a program aimed at the development of catalysts containing a metal centre with coordinated imidazole ligands we have synthesized the title rhodium complex (Niele, Zwikker & Nolte, 1986; Smeets, Sijbesma, Niele, Spek, Smeets & Nolte, 1987). It is the first example of a Rh^{III} complex with an *N*-bonded benzimidazole derivative as a ligand that has been characterized by X-ray methods. The title compound was obtained from a reaction of $RhCl_3$ with 1-methylbenzimidazole in dimethyl sulfoxide (Me_2SO). It resembles the crystal structure of $Rh(Me_2SO)_3Cl_3$ with the oxygen-bonded Me_2SO molecule replaced by the present 1-methylbenzimidazole ligand (Sokol & Porai-Koshits, 1975).

Experimental. Crystals were obtained by recrystallization from Me_2SO. A block-shaped transparent orange crystal 0·20 × 0·25 × 0·37 mm suitable for X-ray diffraction was sealed in a Lindemann-glass capillary to avoid loss of Me_2SO. Enraf–Nonius CAD-4F diffractometer, Zr-filtered Mo $K\alpha$ radiation, unit-cell parameters and their e.s.d.'s were derived from

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Table 1. *Positional and equivalent isotropic thermal parameters for the non-hydrogen atoms with e.s.d.'s in parentheses*

$$U_{\rm eq} = \tfrac{1}{3}\sum_i\sum_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	$U_{\rm eq}$(Å^2)
Rh	0·18411 (3)	0·14874 (3)	0·15467 (2)	0·0304 (1)
Cl(1)	0·0273 (1)	0·1974 (1)	0·1586 (1)	0·0517 (6)
Cl(2)	0·3390 (1)	0·0954 (1)	0·1495 (1)	0·0490 (6)
Cl(3)	0·2062 (1)	0·2142 (1)	0·0530 (1)	0·0553 (6)
S(1)	0·1714 (1)	0·0813 (1)	0·2526 (1)	0·0384 (5)
S(2)	0·2310 (1)	0·2739 (1)	0·2005 (1)	0·0409 (6)
O(1)	0·1592 (3)	−0·0107 (3)	0·2481 (2)	0·053 (2)
O(2)	0·2142 (3)	0·2810 (3)	0·2698 (2)	0·053 (2)
N(1)	0·1393 (3)	0·0396 (3)	0·1052 (2)	0·034 (2)
N(2)	0·1435 (4)	−0·0514 (3)	0·0239 (2)	0·041 (2)
C(1)	0·0591 (4)	−0·0121 (4)	0·1099 (3)	0·034 (2)
C(2)	0·0620 (5)	−0·0687 (4)	0·0583 (3)	0·040 (2)
C(3)	−0·0066 (5)	−0·1298 (4)	0·0491 (3)	0·052 (3)
C(4)	−0·0776 (5)	−0·1341 (4)	0·0947 (4)	0·062 (3)
C(5)	−0·0798 (5)	−0·0792 (4)	0·1472 (4)	0·058 (3)
C(6)	−0·0127 (4)	−0·0166 (4)	0·1559 (4)	0·044 (2)
C(7)	0·1870 (5)	0·0135 (4)	0·0531 (3)	0·036 (2)
C(8)	0·1756 (5)	−0·0969 (4)	−0·0330 (3)	0·056 (3)
C(9)	0·2719 (5)	0·0979 (5)	0·3023 (3)	0·061 (3)
C(10)	0·0820 (5)	0·1238 (4)	0·3028 (3)	0·056 (3)
C(11)	0·1767 (6)	0·3624 (4)	0·1639 (4)	0·073 (3)
C(12)	0·3525 (5)	0·2945 (5)	0·1862 (4)	0·065 (3)
(Me_2SO solvate)				
S(3)	0·4287 (1)	0·4226 (1)	0·4129 (1)	0·0683 (8)
O(3)	0·3721 (4)	0·4956 (3)	0·4373 (3)	0·084 (3)
C(13)	0·4772 (7)	0·3717 (5)	0·4815 (4)	0·092 (4)
C(14)	0·3467 (5)	0·3455 (5)	0·3920 (4)	0·081 (4)

Table 2. *Bond distances* (Å) *and bond angles* (°) *for the non-hydrogen atoms with e.s.d.'s in parentheses*

Rh—Cl(1)	2·340 (2)	S(3)—C(13)	1·764 (9)
Rh—Cl(2)	2·341 (2)	S(3)—C(14)	1·732 (8)
Rh—Cl(3)	2·358 (2)	N(1)—C(1)	1·397 (7)
Rh—S(1)	2·290 (2)	N(1)—C(7)	1·332 (8)
Rh—S(2)	2·286 (2)	N(2)—C(2)	1·377 (9)
Rh—N(1)	2·098 (5)	N(2)—C(7)	1·336 (8)
S(1)—O(1)	1·464 (5)	N(2)—C(8)	1·448 (8)
S(1)—C(9)	1·767 (7)	C(1)—C(6)	1·389 (9)
S(1)—C(10)	1·763 (7)	C(1)—C(2)	1·390 (9)
S(2)—O(2)	1·453 (5)	C(2)—C(3)	1·378 (9)
S(2)—C(11)	1·762 (7)	C(3)—C(4)	1·37 (1)
S(2)—C(12)	1·767 (7)	C(4)—C(5)	1·39 (1)
S(3)—O(3)	1·488 (5)	C(5)—C(6)	1·379 (9)

Cl(1)—Rh—Cl(2)	177·98 (6)	O(2)—S(2)—C(11)	106·8 (3)
Cl(1)—Rh—Cl(3)	90·67 (6)	O(2)—S(2)—C(12)	107·9 (3)
Cl(1)—Rh—S(1)	92·75 (6)	C(11)—S(2)—C(12)	101·7 (4)
Cl(1)—Rh—S(2)	88·58 (6)	O(3)—S(3)—C(13)	106·8 (4)
Cl(1)—Rh—N(1)	90·1 (1)	O(3)—S(3)—C(14)	105·7 (3)
Cl(2)—Rh—Cl(3)	89·65 (6)	C(13)—S(3)—C(14)	98·0 (4)
Cl(2)—Rh—S(1)	86·91 (6)	Rh—N(1)—C(1)	133·5 (4)
Cl(2)—Rh—S(2)	93·43 (6)	C(1)—N(1)—C(7)	106·5 (5)
Cl(2)—Rh—N(1)	87·9 (1)	Rh—N(1)—C(7)	119·6 (4)
Cl(3)—Rh—S(1)	176·53 (6)	C(7)—N(2)—C(8)	127·0 (6)
Cl(3)—Rh—S(2)	87·21 (7)	C(2)—N(2)—C(8)	125·4 (5)
Cl(3)—Rh—N(1)	88·1 (1)	C(2)—N(2)—C(7)	107·6 (5)
S(1)—Rh—S(2)	93·39 (7)	N(1)—C(1)—C(2)	107·3 (5)
S(1)—Rh—N(1)	91·4 (1)	N(1)—C(1)—C(6)	131·8 (6)
S(2)—Rh—N(1)	175·1 (1)	C(2)—C(1)—C(6)	120·8 (6)
Rh—S(1)—O(1)	114·4 (2)	N(2)—C(2)—C(3)	130·7 (6)
Rh—S(1)—C(9)	112·3 (2)	N(2)—C(2)—C(1)	107·0 (5)
Rh—S(1)—C(10)	113·4 (2)	C(1)—C(2)—C(3)	122·3 (6)
O(1)—S(1)—C(9)	106·1 (3)	C(2)—C(3)—C(4)	116·8 (6)
O(1)—S(1)—C(10)	109·3 (3)	C(3)—C(4)—C(5)	121·3 (6)
C(9)—S(1)—C(10)	100·1 (3)	C(4)—C(5)—C(6)	122·2 (7)
Rh—S(2)—O(2)	115·2 (2)	C(1)—C(6)—C(5)	116·6 (7)
Rh—S(2)—C(11)	112·4 (3)	N(1)—C(7)—N(2)	111·6 (6)
Rh—S(2)—C(12)	111·7 (3)		

the angular settings of 12 reflections with $9{\cdot}9 < \theta < 13{\cdot}2°$. Intensity data of 4499 unique reflections were collected within one octant of the reflection sphere [$0 \le h \le 16$; $0 \le k \le 18$; $0 \le l \le 24$; $0{\cdot}99 < \theta < 25{\cdot}0°$] in $\omega/2\theta$ scan mode with $\Delta\omega = (0{\cdot}55 + 0{\cdot}35\tan\theta)°$. Three reference reflections [600 (e.s.d. = 0·78%); 040 (e.s.d. = 1·11%); 0,0,10 (e.s.d. = 0·72%)], measured every hour showed a linear decay of 1·9% during the 84 h of X-ray exposure time. The intensity data were corrected for this small decay and for Lp but not for absorption. Standard deviations in the intensities based on counting statistics were increased according to an analysis of the excess variance of the reference reflections: $\sigma^2(I) = \sigma^2_{\rm cs}(I) + (0{\cdot}0184I)^2$ (McCandlish, Stout & Andrews, 1975) resulting in 2554 reflections with $I > 2\sigma(I)$. Space group *Pbca* derived from the observed systematic absences: $0kl$, $k = 2n+1$; $h0l$, $l = 2n+1$ and $hk0$, $h = 2n+1$.

The structure was solved by standard Patterson (*SHELXS*86; Sheldrick, 1986) and subsequent difference Fourier methods. H atoms were introduced on calculated positions (C—H = 0·98 Å) and included in weighted full-matrix refinement (on F) riding on their carrier atom with one common isotropic thermal parameter. All non-H atoms were refined with anisotropic thermal parameters. Convergence with 257 parameters was reached at $R = 0{\cdot}0440$, $wR = 0{\cdot}0335$, $w = 1/\sigma^2(F)$, $S = 1{\cdot}46$, $(\Delta/\sigma)_{\rm ave.} = 0{\cdot}058$. The final difference Fourier synthesis revealed max. and min. residual densities of 0·94 and −0·53 e Å^{-3} near the Rh atom.

Scattering factors from Cromer & Mann (1968); anomalous-dispersion corrections from Cromer & Liberman (1970). Calculations performed with *SHELX*76 (Sheldrick, 1976) and the *EUCLID* package (geometry calculations and illustrations) (Spek, 1982) on the CDC Cyber-855 of the University of Utrecht.

Discussion. Refined atomic coordinates and equivalent isotropic thermal parameters of the non-hydrogen atoms are given in Table 1.* Bond lengths and bond angles are listed in Table 2. The molecular structure of the title compound and the adopted atom numbering are presented in Fig. 1.

The orthorhombic unit cell contains eight discrete molecules of the Rh$^{\rm III}$ complex and eight Me_2SO

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* Lists of structure factors, anisotropic thermal parameters, H-atom parameters, torsion angles and geometrical data concerning H atoms have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44284 (30 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

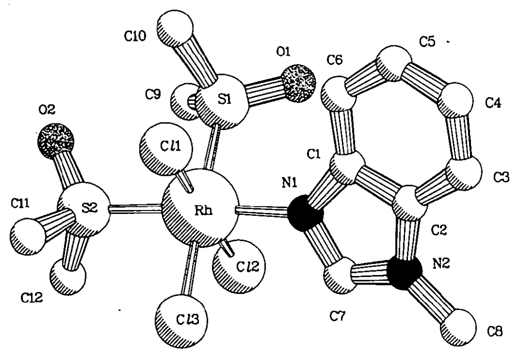

Fig. 1. *PLUTO* (*EUCLID* version) drawing of the title compound with the adopted atom numbering. Hydrogen atoms and the Me_2SO molecule of crystallization are omitted for clarity.

molecules of crystallization. The Rh atom is octahedrally coordinated by two S atoms of Me_2SO 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_2SO 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.

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

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Abstract. $[Cu(C_{10}H_9N_4O_2S)_2(NH_3)_2]$, $M_r = 596{\cdot}15$, 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, $\frac{1}{2}-z$), $a = 13{\cdot}915$ (5), $b = 14{\cdot}356$ (5), $c = 12{\cdot}659$ (5) Å, $V = 2528{\cdot}81$ Å^3, $Z = 4$, $D_m = 1{\cdot}55$ (1), $D_x = 1{\cdot}566$ Mg m^{-3}, λ(Mo $K\alpha$) $= 0{\cdot}71069$ Å, $\mu = 1{\cdot}11$ mm^{-1}, $F(000) = 1228$, $T =$

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* Copper sulphadiazine diammoniate.

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