Crystal and Molecular Structure of Trichloro(dimethyl sulphoxide)bispyridinerhodium(III)

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The structure of the title complex has been determined by direct methods from *X*-ray diffractometer data. Crystals are monoclinic, space group $P2_1/n$, with $a = 12.621(5)$, $b = 8.805(3)$, $c = 30.357(7)$ Å, $\beta = 101.56(3)°$, $Z = 8$. 1 779 Observed reflections were used and the structure refined by least squares to R 0.048.

The structure consists of discrete molecules of [$RhCl_3$(dmso)(py)$_2$] in which the Rh atoms are co-ordinated, in a nearly regular octahedron, by three meridional chlorine atoms, two *cis*-nitrogen atoms from the pyridine, and the sulphur atom of the dimethyl sulphoxide. The molecules are linked by van der Waals interactions.

DURING an investigation of the biological and antitumour activity of co-ordination compounds, the structure of [$RhCl_3$(dmso)(py)$_2$] has been determined. This complex shows a remarkable activity against P 388 leukemia (in mice) and KB carcinoma (test *in vitro*).[1] Recent studies have shown that, besides the thermodynamic and kinetic stability of the active complexes,[2] steric factors play an important role in their mechanism of action. For this reason a comparison between the molecular geometry of [$RhCl_3$(dmso)(py)$_2$] and those of the well known active complexes of platinum(II) seemed interesting.

EXPERIMENTAL

Crystal Data.—[$RhCl_3$(dmso)(py)$_2$], $C_{12}H_{16}Cl_3N_2ORhS$, $M = 445.60$, Monoclinic, $a = 12.621(5)$, $b = 8.805(3)$, $c = 30.357(7)$ Å, $\beta = 101.56(3)°$, $U = 3\,306.8$ Å^3, $Z = 8$, $D_c = 1.79$ g cm^{-3}, λ(Mo-$K_{\alpha1}$) = 0.7093 Å, μ(Mo-$K_{\alpha1}$) = 16.2 cm^{-1}. Space group $P2_1/n$. There are two independent molecules in the asymmetric unit.

Data Collection.—The compound was prepared by the method of ref. 3. A prismatic crystal, elongated along the b axis, with dimensions $0.50 \times 0.08 \times 0.08$ mm was mounted on a Philips automatic diffractometer.

The 'peak hunting' routine,[4] applied in two different zones of the reciprocal lattice, yielded two independent sets of 25 reflections, which gave the same monoclinic cell. A least-squares refinement of the lattice constants was performed on 45 reflections whose θ values were accurately centred on the diffractometer. Intensity data were collected with the following experimental conditions: ω—2θ scan, scan speed 0.07 °s^{-1}, scan width 1.2°, stationary-counter background counts 8.5 s (half total scan time) at each end of scan range, take-off angle 4.5°, graphite-monochromatized Mo radiation. After correction for the background, the standard deviation $\sigma(I)$ of the corrected intensity was estimated according to the expression: $\sigma(I) = [P + B_1 + B_2 + (KI)^2]^{1/2}$, where P is the total peak count and B_1 and B_2 the background counts. The value of K, determined by a least-squares analysis of the intensities of three reflections monitored periodically, was 0.005. During data collection no appreciable variation in the standard reflections was observed. In the range $4° < 2\theta < 40°$ 3 378 independent reflections were measured, of which 1 779 having $I > 3\sigma(I)$ were considered observed. The measured intensities were corrected for Lorentz-polarization factors; no correction was made for absorption effects since transmission factors, calculated by means of the program AGNOSTX, ranged between 0.85 and 0.88.

Structure Determination.—The structure was solved by direct methods, by use of the program MULTAN[5] which gave unambiguously the positions of the atoms forming the co-ordination polyhedra in the two independent molecules. Two isotropic least-squares cycles of refinement on these atom positions, followed by an electron-density synthesis, gave the positions of the remaining atoms, except hydrogen, these being introduced in calculated positions in the last stages of refinement. A further cycle of isotropic refinement and two cycles of refinement with anisotropic temperature factors for rhodium, chlorine, sulphur, oxygen, and nitrogen gave R 0.048. Hydrogen atoms were assigned a temperature factor equal to that of the carbon atom to which they are bound. The function minimized in the refinement was $\Sigma w(|F_o| - |F_c|)^2$ with weights from counting statistics taken as $4F_o^2/\sigma^2(F_o^2)$. The weighted factor R' $\{R' = [\Sigma w(|F_o| - |F_c|)^2/\Sigma wF_o^2]^{1/2}\}$ was 0.042. The mean shift-to-error ratio in the last cycle was 0.37. Atomic scattering factors were taken from ref. 6, those for rhodium, chlorine, and sulphur being corrected for both the real and imaginary parts of the anomalous dispersion terms.[7] Besides the programs already mentioned, the '*X*-Ray '72' system[8] adapted for use on the CII 10070 computer of the University of Florence was used for all calculations. Atomic parameters with their standard deviations in the last significant digits, calculated from the inverse matrix, are reported in Table 1.

The list of atomic parameters shows clearly that the co-ordinates of corresponding atoms in the two independent molecules are strongly correlated. In fact, for each pair of atoms, the y co-ordinates are the same within a few σ deviations, whereas the sum of the z co-ordinates is 0.5. It can easily be shown that this causes additional extinctions of $0kl$ reflections for k odd.

No immediate relationship is apparent for the x co-ordinates, unless one chooses a new cell defined by the vectors $\boldsymbol{a}$, $\boldsymbol{b}$, $\boldsymbol{c}'$, where $\boldsymbol{c}' = 2\boldsymbol{c} + \boldsymbol{a}$. In this new cell, which is pseudo-orthorhombic ($c' = 59.484$ Å, $\beta' = 89.56°$), the two independent molecules are related by a sort of glide plane perpendicular to c', at $z = \frac{1}{8}$, with a translation of $\frac{1}{4}$

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[1] P. Colamarino, P. L. Orioli, P. Nannelli, and B. P. Block, *Atti VIII Convegno Nazionale Chim. Inorg.*, Sept. 1975, Iesolo, Italy.

[2] M. J. Cleare, *Co-ordination Chem. Rev.*, 1974, **12**, 349.

[3] Y. N. Kukushkin and N. D. Rubtsova, *Russ. J. Inorg. Chem.*, 1969, **14**, 980.

[4] Philips, *Serving Science and Industry*, 1972, **18**, 22.

[5] MULTAN, program written by P. Main, M. M. Woolfson, and G. Germain, *Acta Cryst*, 1971, **A27**, 368.

[6] D. T. Cromer and J. T. Waber, *Acta Cryst.*, 1965, **18**, 104.

[7] 'International Tables for *X*-Ray Crystallography,' vol. III, Kynoch Press, Birmingham, 1962.

[8] '*X*-Ray '72,' Technical Report TR 192, 1972, University of Maryland, U.S.A., eds. J. M. Stewart, F. A. Kundell, and J. C. Baldwin.

along *a*. The co-ordinates of the corresponding atoms in the two molecules are then related as follows:

$$\begin{vmatrix} x' \\ y' \\ z' \end{vmatrix} = \begin{vmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \bar{1} \end{vmatrix} \begin{vmatrix} x \\ y \\ z \end{vmatrix} + \begin{vmatrix} \frac{1}{4} \\ 0 \\ \frac{1}{4} \end{vmatrix}$$

The mean deviation from this relationship for corresponding pairs of atomic co-ordinates amounts to *ca.* 3σ with a maximum of 36σ for the *x* co-ordinate of the rhodium atoms. Examination of the equivalent reflections rules out any possibility of assignment of the compounds to the orthorhombic system. Structure factors are listed in Supplementary Publication No. SUP 21607 (4 pp., 1 microfiche).[*]

TABLE 1

Positional parameters ($\times 10^4$), thermal parameters [*] ($Å^2 \times 10^3$), and estimated standard deviations

Atom	x/a	y/b	z/c	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Rh(1)	5 524(1)	2 340(2)	1 194(1)	32(1)	31(1)	22(1)	0(1)	4(1)	−2(1)
Rh(2)	4 357(1)	2 355(2)	3 788(1)	36(1)	30(1)	25(1)	0(1)	10(1)	−2(1)
Cl(1)	7 017(4)	1 027(5)	1 607(2)	42(3)	38(3)	32(3)	1(3)	4(2)	3(3)
Cl(2)	4 876(4)	87(5)	838(2)	42(3)	41(3)	34(3)	−2(3)	3(2)	−9(3)
Cl(3)	4 082(4)	3 645(5)	770(2)	43(3)	48(3)	34(3)	9(3)	−2(3)	2(3)
Cl(4)	5 465(4)	1 057(5)	3 380(2)	46(3)	36(3)	41(3)	4(3)	15(3)	−4(3)
Cl(5)	4 059(4)	84(5)	4 144(2)	51(3)	38(3)	38(3)	0(3)	18(3)	4(3)
Cl(6)	3 306(4)	3 647(5)	4 213(2)	55(4)	48(3)	32(3)	10(3)	17(3)	1(3)
S(1)	4 490(4)	1 870(5)	1 717(2)	38(3)	46(3)	34(3)	−7(3)	13(3)	−2(3)
S(2)	2 814(4)	1 904(5)	3 267(2)	38(3)	40(3)	38(3)	−3(3)	12(3)	0(3)
O(1)	4 500(9)	3 091(13)	2 053(4)	67(9)	57(9)	29(8)	−13(7)	15(6)	−28(7)
O(2)	2 454(9)	3 115(14)	2 944(4)	64(9)	63(9)	40(9)	3(7)	3(7)	26(8)
N(1)	6 077(10)	4 323(15)	1 493(4)	32(9)	37(10)	33(10)	8(7)	13(7)	13(8)
N(2)	6 446(10)	2 811(15)	713(4)	41(9)	44(10)	19(8)	−8(8)	4(7)	7(7)
N(3)	4 615(9)	4 355(14)	3 480(4)	35(9)	32(9)	26(9)	−1(7)	9(7)	−13(8)
N(4)	5 698(10)	2 814(14)	4 269(4)	47(9)	31(9)	33(9)	−3(7)	16(7)	−2(8)

Atom	x/a	y/b	z/c	U	Atom	x/a	y/b	z/c	U
C(1)	6 009(13)	5 642(19)	1 275(6)	42(5)	C(13)	4 749(13)	5 674(18)	3 704(6)	39(5)
C(2)	6 396(13)	7 005(19)	1 455(6)	43(5)	C(14)	4 937(13)	7 052(19)	3 522(6)	43(5)
C(3)	6 934(13)	7 033(19)	1 899(6)	41(5)	C(15)	5 072(14)	7 013(20)	3 079(6)	53(6)
C(4)	7 013(14)	5 696(21)	2 141(6)	51(6)	C(16)	4 940(13)	5 677(20)	2 835(6)	44(5)
C(5)	6 630(13)	4 374(19)	1 933(6)	41(5)	C(17)	4 713(13)	4 386(19)	3 039(6)	44(5)
C(6)	7 456(14)	3 374(20)	833(6)	50(6)	C(18)	6 594(14)	3 404(20)	4 173(6)	50(6)
C(7)	8 033(14)	3 818(21)	510(7)	55(6)	C(19)	7 505(16)	3 849(22)	4 495(7)	64(6)
C(8)	7 567(15)	3 644(19)	69(5)	50(5)	C(20)	7 470(15)	3 644(20)	4 950(7)	64(6)
C(9)	6 555(14)	2 981(20)	−69(6)	51(5)	C(21)	6 570(14)	2 959(20)	5 048(6)	50(6)
C(10)	5 987(12)	2 602(20)	266(5)	41(5)	C(22)	5 698(13)	2 584(21)	4 717(6)	49(5)
C(11)	3 118(14)	1 481(20)	1 463(6)	53(6)	C(23)	1 694(13)	1 483(19)	3 513(6)	46(5)
C(12)	4 853(14)	108(22)	1 989(6)	64(6)	C(24)	2 904(14)	203(21)	2 962(6)	61(6)
H(1) [†]	5 624	5 632	951	42	H(13)	4 701	5 672	4 028	39
H(2)	6 299	7 946	1 253	43	H(14)	4 985	8 025	3 690	43
H(3)	7 264	7 981	2 042	41	H(15)	5 255	7 962	2 928	53
H(4)	7 360	5 694	2 465	51	H(16)	5 012	5 655	2 514	44
H(5)	6 752	3 417	2 111	41	H(17)	4 635	3 432	2 861	44
H(6)	7 786	3 519	1 157	50	H(18)	6 624	3 560	3 850	50
H(7)	8 794	4 212	600	55	H(19)	8 158	4 278	4 399	64
H(8)	7 967	3 996	−165	50	H(20)	8 074	4 002	5 191	64
H(9)	6 248	2 813	−393	51	H(21)	6 563	2 772	5 372	50
H(10)	5 236	2 182	179	41	H(22)	5 056	2 118	4 810	49
1H(11)	3 012	797	1 181	53	1H(23)	1 536	469	3 365	46
2H(11)	2 752	928	1 685	53	2H(23)	1 883	1 396	3 855	46
3H(11)	2 716	2 438	1 370	53	3H(23)	1 074	2 214	3 434	46
1H(12)	5 459	−601	1 990	64	1H(23)	2 981	−600	3 139	61
2H(12)	4 912	297	2 321	64	2H(24)	2 243	54	2 720	61
3H(12)	4 209	−592	1 887	64	3H(24)	3 556	244	2 814	61

[*] Anisotropic thermal factors are of the form: $\exp[-2\pi^2(U_{11}h^2a^{*2} + U_{22}k^2b^{*2} + U_{33}l^2c^{*2} + 2U_{12}hka^*b^* + 2U_{13}hla^*c^* + 2U_{23}klb^*c^*)]$. [†] Hydrogen atoms numbered according to the carbon atom to which they are attached.

DISCUSSION AND DESCRIPTION OF THE STRUCTURE

The structure consists of discrete molecules of $[\text{RhCl}_3(\text{dmso})(\text{py})_2]$ (Figure). In the unit cell, as already mentioned, there are two independent molecules, in which the differences between corresponding bond lengths and angles are all within 3 σ (Table 2). The rhodium atom is in the centre of a fairly regular octahedron, whose vertices are formed by three chlorine atoms coplanar with the metal, two nitrogen atoms of the pyridine rings in *cis*-position, and a sulphur atom of the dimethyl sulphoxide group. Rh–Cl and Rh–N distances, which do not show significant discrepancies among themselves, are in agreement with analogous distances found in octahedral Rh^{III} complexes.[9-11] Rh–N distances show also that dmso does not exert any appreciable *trans*-influence on these bonds. Comparison of the Rh–Cl and Rh–N distances with corresponding distances in platinum(II) complexes,

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[*] See Notice to Authors No. 7, in *J.C.S. Dalton*, 1975, Index issue. (Items less than 10 pp. are supplied as full-size copies.)

[9] R. Mason and A. D. C. Towl, *J. Chem. Soc.* (*A*), 1970, 1601.

[10] G. C. Dobinson, R. Mason, and D. R. Russell, *Chem. Comm.*, 1967, 62.

[11] J. A. Evans, D. R. Russell, A. Bright, and B. L. Shaw, *Chem. Comm.*, 1971, 841.

which have been shown to possess anticancer activity, is interesting. In fact, in the well known and widely studied square-planar *cis*-[Pt(NH$_3$)$_2$Cl$_2$], mean Pt–Cl and Pt–N distances are respectively 2.33(1) and 2.01(4) Å.[12] In *cis*-[Pt(py)$_2$Cl$_2$], which shows activity against Ehrlich ascites tumour,[13] mean Pt–Cl and Pt–N are respectively 2.296(5) and 2.02(1) Å.[14] Another common structural feature of all these active complexes is the *cis*-position of the chlorine atoms. This evidence shows that the geometric requirements for antitumour activity in complexes are rather strict and that stereochemistry plays an essential role in their mechanism of action.

TABLE 2

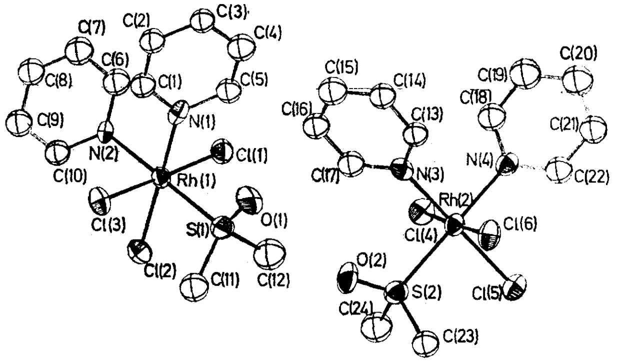
Bond lengths (Å) and angles (°), with estimated standard deviations in parentheses

(*a*) Distances

Rh(1)–Cl(1)	2.348(4)	Rh(2)–Cl(4)	2.342(5)
Rh(1)–Cl(2)	2.331(5)	Rh(2)–Cl(5)	2.343(5)
Rh(1)–Cl(3)	2.314(5)	Rh(2)–Cl(6)	2.325(5)
Rh(1)–N(1)	2.028(13)	Rh(2)–N(3)	2.053(13)
Rh(1)–N(2)	2.082(13)	Rh(2)–N(4)	2.041(11)
Rh(1)–S(1)	2.284(5)	Rh(2)–S(2)	2.283(4)
S(1)–O(1)	1.48(1)	S(2)–O(2)	1.46(1)
S(1)–C(11)	1.78(2)	S(2)–C(23)	1.76(2)
S(1)–C(12)	1.78(2)	S(2)–C(24)	1.78(2)
N(1)–C(1)	1.33(2)	N(3)–C(13)	1.34(2)
C(1)–C(2)	1.37(2)	C(13)–C(14)	1.38(2)
C(2)–C(3)	1.38(2)	C(14)–C(15)	1.39(3)
C(3)–C(4)	1.38(2)	C(15)–C(16)	1.38(2)
C(4)–C(5)	1.37(2)	C(16)–C(17)	1.35(2)
C(5)–N(1)	1.38(2)	C(17)–N(3)	1.37(2)
N(2)–C(6)	1.35(2)	N(4)–C(18)	1.33(2)
C(6)–C(7)	1.39(3)	C(18)–C(19)	1.41(2)
C(7)–C(8)	1.36(3)	C(19)–C(20)	1.40(3)
C(8)–C(9)	1.39(2)	C(20)–C(21)	1.37(3)
C(9)–C(10)	1.39(3)	C(21)–C(22)	1.37(2)
C(10)–N(2)	1.37(2)	C(22)–N(4)	1.37(2)

(*b*) Angles

Cl(1)–Rh(1)–Cl(2)	89.7(2)	Cl(4)–Rh(2)–Cl(5)	89.6(2)
Cl(1)–Rh(1)–Cl(3)	178.2(3)	Cl(4)–Rh(2)–Cl(6)	178.1(2)
Cl(1)–Rh(1)–N(1)	91.2(3)	Cl(4)–Rh(2)–N(3)	90.9(4)
Cl(1)–Rh(1)–N(2)	88.3(3)	Cl(4)–Rh(2)–N(4)	88.7(4)
Cl(1)–Rh(1)–S(1)	92.8(2)	Cl(4)–Rh(2)–S(2)	93.8(2)
Cl(2)–Rh(1)–Cl(3)	90.2(2)	Cl(5)–Rh(2)–Cl(6)	90.1(2)
Cl(2)–Rh(1)–N(1)	178.9(4)	Cl(5)–Rh(2)–N(3)	179.5(4)
Cl(2)–Rh(1)–N(2)	92.3(4)	Cl(5)–Rh(2)–N(4)	91.5(4)
Cl(2)–Rh(1)–S(1)	88.3(2)	Cl(5)–Rh(2)–S(2)	88.7(2)
Cl(3)–Rh(1)–N(1)	88.9(3)	Cl(6)–Rh(2)–N(3)	89.4(4)
Cl(3)–Rh(1)–N(2)	89.9(3)	Cl(6)–Rh(2)–N(4)	89.4(4)
Cl(3)–Rh(1)–S(1)	88.9(2)	Cl(6)–Rh(2)–S(2)	88.1(2)
N(1)–Rh(1)–N(2)	87.2(5)	N(3)–Rh(2)–N(4)	88.3(5)
N(1)–Rh(1)–S(1)	92.3(4)	N(3)–Rh(2)–S(2)	91.5(2)
N(2)–Rh(1)–S(1)	178.7(6)	N(4)–Rh(2)–S(2)	177.5(5)
Rh(1)–S(1)–O(1)	114.7(5)	Rh(2)–S(2)–O(2)	116.4(5)
Rh(1)–S(1)–C(11)	112.1(7)	Rh(2)–S(2)–C(23)	112.9(6)
Rh(1)–S(1)–C(12)	110.6(7)	Rh(2)–S(2)–C(24)	111.8(6)
O(1)–S(1)–C(11)	108.0(8)	O(2)–S(2)–C(23)	105.6(8)
O(1)–S(1)–C(12)	110.6(8)	O(2)–S(2)–C(24)	108.3(8)
C(11)–S(1)–C(12)	99.7(8)	C(23)–S(2)–C(24)	100.5(9)
Rh(1)–N(1)–C(1)	123(1)	Rh(2)–N(3)–C(13)	122(1)
Rh(1)–N(1)–C(5)	122(1)	Rh(2)–N(3)–C(17)	121(1)
C(1)–N(1)–C(5)	115(1)	C(13)–N(3)–C(17)	117(1)
N(1)–C(1)–C(2)	126(1)	N(3)–C(13)–C(14)	125(2)
C(1)–C(2)–C(3)	118(2)	C(13)–C(14)–C(15)	116(2)
C(2)–C(3)–C(4)	118(1)	C(14)–C(15)–C(16)	121(2)
C(3)–C(4)–C(5)	120(2)	C(15)–C(16)–C(17)	119(2)
C(4)–C(5)–N(1)	123(2)	C(16)–C(17)–N(3)	122(2)
Rh(1)–N(2)–C(6)	121(1)	Rh(2)–N(4)–C(18)	123(1)
Rh(1)–N(2)–C(10)	119(1)	Rh(2)–N(4)–C(22)	121(1)
C(6)–N(2)–C(10)	120(1)	C(18)–N(4)–C(22)	116(1)
N(2)–C(6)–C(7)	121(2)	N(4)–C(18)–C(19)	125(2)
C(6)–C(7)–C(8)	119(2)	C(18)–C(19)–C(20)	118(2)
C(7)–C(8)–C(9)	122(2)	C(19)–C(20)–C(21)	117(2)
C(8)–C(9)–C(10)	117(2)	C(20)–C(21)–C(22)	122(2)
C(9)–C(10)–N(2)	121(1)	C(21)–C(22)–N(4)	122(2)



ORTEP diagram of [RhCl$_3$(dmso)(py)$_2$], showing the atom labelling and the mutual orientation of the two independent molecules

The dmso group co-ordinates to the metal through sulphur, which is in agreement with the soft character of the rhodium atom. With first-row transition metals, however, dmso binds through oxygen.[15-17] Bond angles and S–C distances in dmso are not too different from the values reported for the crystalline free ligand.[18] However, S–O distances [1.48(1) and 1.46(1) Å] are significantly shorter than that in dmso itself [1.513(5) Å].[18]

TABLE 3

Intermolecular distances <3.70 Å

Cl(1) ··· C(2$^{\mathrm{I}}$)	3.64(2)	C(6) ··· C(14$^{\mathrm{V}}$)	3.67(2)
Cl(1) ··· C(3$^{\mathrm{I}}$)	3.64(2)	C(22) ··· C(2$^{\mathrm{V}}$)	3.68(3)
Cl(2) ··· C(2$^{\mathrm{I}}$)	3.62(2)	Cl(3) ··· C(23$^{\mathrm{VI}}$)	3.58(2)
Cl(4) ··· C(14$^{\mathrm{I}}$)	3.64(2)	Cl(6) ··· C(11$^{\mathrm{VI}}$)	3.49(2)
Cl(4) ··· C(15$^{\mathrm{I}}$)	3.69(2)	O(1) ··· C(23$^{\mathrm{VI}}$)	3.62(2)
Cl(5) ··· C(14$^{\mathrm{I}}$)	3.58(2)	O(1) ··· C(24$^{\mathrm{VI}}$)	3.55(2)
Cl(3) ··· C(9$^{\mathrm{II}}$)	3.65(2)	O(2) ··· C(11$^{\mathrm{VI}}$)	3.62(2)
Cl(3) ··· C(20$^{\mathrm{III}}$)	3.52(2)	O(2) ··· C(12$^{\mathrm{VI}}$)	3.44(2)
Cl(6) ··· C(8$^{\mathrm{IV}}$)	3.56(2)	O(2) ··· C(24$^{\mathrm{VI}}$)	3.26(2)
Cl(6) ··· C(9$^{\mathrm{IV}}$)	3.69(2)	C(1) ··· C(23$^{\mathrm{VI}}$)	3.67(2)
Cl(4) ··· C(3$^{\mathrm{V}}$)	3.65(2)	C(13) ··· C(11$^{\mathrm{VI}}$)	3.62(2)

Roman numeral superscripts refer to the following equivalent positions relative to the reference molecule at x, y, z:

I	$x, y - 1, z$	IV	$x - 1/2, 1/2 - y, 1/2 + z$
II	$1 - x, 1 - y, -z$	V	$3/2 - x, y - 1/2, 1/2 - z$
III	$x - 1/2, 1/2 - y, z - 1/2$	VI	$1/2 - x, 1/2 + y, 1/2 - z$

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This can be accounted for by an increase of the triple-bond character of the S–O bond, as suggested also by other authors.[19,20] Bond lengths and angles in the pyridine rings are as expected. These rings form with, the plane defined by atoms Rh, N, N′, S, Cl, angles of 55.5 and 42.9° in one molecule and 55.8 and 41.7° in the other. The oxygen atoms of the dmso groups also lie in this plane. Table **3** lists shortest intermolecular contacts. It appears that normal van der Waals attractions are the only packing forces in the structure.

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