Table 1. Crystal data and structure refinement for JJR2 $RuCl_3(DMSO)(TMEDA)$.

Empirical formula	$C_8H_{22}Cl_3N_2ORuS$
Formula weight	401.76
Crystallization Solvent	$EtOH/H_2O$
Crystal Habit	Rhomb
Crystal size	0.48 x 0.39 x 0.33 mm^3
Crystal color	Reddish-orange

Data Collection

Type of diffractometer	CAD-4	
Wavelength	0.71073 Å MoKα	
Data Collection Temperature	85 K	
Theta range for reflections used in lattice determination	21 to 28°	
Unit cell dimensions	a = 14.086(4) Å b = 8.716(2) Å c = 24.444(4) Å	α= 90° β= 97.13(2)° γ= 90°
Volume	2977.9(12) $Å^3$	
Z	8	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Density (calculated)	1.792 Mg/m^3	
F(000)	1624	
Theta range for data collection	1.50 to 30°	
Index ranges	-19<=h<=19, -12<=k<=11, 0<=l<=34	
Data collection scan type	Ω–scans	
Reflections collected	16742	
Independent reflections	8665 [R_{int}= 0.021; GOF_{merge}= 1.17]	
Absorption coefficient	1.715 mm^{-1}	
Absorption correction	ψ-scan (North, Phillips & Matthews, 1968)	
Max. and min. transmission	1.08 and 0.91	
Number of standards	3 reflections measured every 75min.	
Variation of standards	-0.31%.	

Table 1 (cont.)

Structure solution and Refinement

Structure solution program	SHELXS-97 (Sheldrick, 1990)
Primary solution method	direct methods
Secondary solution method	difference map
Hydrogen placement	geometrical
Structure refinement program	SHELXL-97 (Sheldrick, 1997)
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8665 / 0 / 450
Treatment of hydrogen atoms	mixed
Goodness-of-fit on F^2	1.727
Final R indices [$I>2\sigma(I)$]	R1 = 0.0362, wR2 = 0.0663
R indices (all data)	R1 = 0.0466, wR2 = 0.0680
Type of weighting scheme used	calc
Weighting scheme used	$w=1/\sigma^2(F_o^2)$
Max shift/error	0.008
Average shift/error	0.000
Largest diff. peak and hole	1.611 and -1.026 e.Å^{-3}

Special Refinement Details

Background functions of 2θ were not used due to a high internal GOF and no improvement in modelling the data.

There are two molecules in the asymmetric unit. In one of these the TMEDA ligand is disordered. Figures 3 and 4 show how this disorder accompanies the position of the O atom of the DMSO. In the non-disordered molecule, the sulfur-oxygen bond is approximately collinear with the N1A-C1A bond; in the disordered molecule where there are two orientations of the N-C bond (N1B-C1B1, N1B-C1B2), the sulfur-oxygen bond bisects the angle between these two orientations. The disorder was finally modelled by splitting C1B into two components with hydrogen atoms at calculated positions; the two sites refined to a relative population of 0.59(1):0.41(2). The two methyl carbons C2B and C4B are also seriously affected by this disorder but were not split into separate positions. One of the chloride ligands also has a slightly irregular displacement ellipsoid.

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for JJR2 $RuCl_3$(DMSO)(TMEDA). U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ru(A)	1709(1)	5092(1)	1316(1)	9(1)
Cl(1A)	3251(1)	5297(1)	1801(1)	17(1)
Cl(2A)	1574(1)	2531(1)	1597(1)	21(1)
Cl(3A)	197(1)	4870(1)	810(1)	18(1)
N(1A)	1091(2)	5942(3)	2044(1)	18(1)
N(2A)	1686(2)	7536(2)	1099(1)	18(1)
C(1A)	1296(2)	7595(4)	2055(1)	27(1)
C(2A)	1072(2)	8251(3)	1489(1)	25(1)
C(3A)	1546(2)	5235(4)	2574(1)	28(1)
C(4A)	51(2)	5655(4)	2032(1)	25(1)
C(5A)	2646(2)	8287(4)	1164(2)	27(1)
C(6A)	1253(3)	7909(4)	526(1)	29(1)
S(A)	2429(1)	4278(1)	577(1)	19(1)
O(A)	2871(2)	5475(3)	264(1)	39(1)
C(7A)	3332(2)	2886(4)	778(1)	27(1)
C(8A)	1656(2)	3142(4)	107(1)	32(1)
Ru(B)	7000(1)	95(1)	1277(1)	10(1)
Cl(1B)	6839(1)	104(1)	310(1)	31(1)
Cl(2B)	7666(1)	-2375(1)	1295(1)	20(1)
Cl(3B)	7088(1)	112(1)	2236(1)	20(1)
N(1B)	8424(2)	1127(3)	1317(1)	37(1)
N(2B)	6536(2)	2503(2)	1265(1)	21(1)
C(1B1)[a]	8138(4)	2816(6)	1089(2)	23(1)
C(1B2)[b]	8348(5)	2708(7)	1539(3)	18(2)
C(2B)	7448(3)	3379(4)	1306(3)	84(2)
C(3B)	8972(3)	680(5)	874(2)	40(1)
C(4B)	9059(3)	779(10)	1829(2)	94(3)
C(5B)	5933(2)	2984(4)	753(1)	25(1)
C(6B)	5982(4)	2943(5)	1724(2)	52(1)
S(B)	5509(1)	-983(1)	1237(1)	15(1)
O(B)	4685(1)	60(2)	1239(1)	28(1)
C(7B)	5259(2)	-2238(4)	662(1)	27(1)
C(8B)	5459(2)	-2342(4)	1776(1)	24(1)

[a] Population 0.59(1)
[b] Population 0.41(1)

Table 3. Bond lengths [Å] and angles [°] for JJR2 $RuCl_3(DMSO)(TMEDA)$.

Ru(A)-N(2A)	2.194(2)	C(1B1)-C(2B)	1.263(7)
Ru(A)-N(1A)	2.204(2)	C(1B1)-H(1BA)	0.9900
Ru(A)-S(A)	2.2912(8)	C(1B1)-H(1BB)	0.9900
Ru(A)-Cl(3A)	2.3340(9)	C(1B2)-C(2B)	1.447(7)
Ru(A)-Cl(1A)	2.3497(9)	C(1B2)-C(4B)	2.039(11)
Ru(A)-Cl(2A)	2.3503(8)	C(1B2)-H(1BC)	0.9900
N(1A)-C(1A)	1.469(4)	C(1B2)-H(1BD)	0.9900
N(1A)-C(4A)	1.483(4)	C(2B)-H(2BA)	0.9900
N(1A)-C(3A)	1.505(4)	C(2B)-H(2BB)	0.9900
N(2A)-C(5A)	1.493(4)	C(3B)-H(3BA)	0.90(4)
N(2A)-C(6A)	1.492(4)	C(3B)-H(3BB)	0.98(3)
N(2A)-C(2A)	1.500(4)	C(3B)-H(3BC)	0.91(4)
C(1A)-C(2A)	1.494(5)	C(4B)-H(4BA)	1.01(6)
C(1A)-H(1AA)	0.93(3)	C(4B)-H(4BB)	0.63(6)
C(1A)-H(1AB)	1.01(4)	C(4B)-H(4BC)	0.74(6)
C(2A)-H(2AA)	1.10(3)	C(5B)-H(5BA)	0.92(3)
C(2A)-H(2AB)	0.90(4)	C(5B)-H(5BB)	0.99(4)
C(3A)-H(3AA)	0.97(3)	C(5B)-H(5BC)	0.94(4)
C(3A)-H(3AB)	1.08(3)	C(6B)-H(6BA)	1.02(4)
C(3A)-H(3AC)	0.97(4)	C(6B)-H(6BB)	0.93(5)
C(4A)-H(4AA)	1.03(4)	C(6B)-H(6BC)	0.94(4)
C(4A)-H(4AB)	0.98(3)	S(B)-O(B)	1.474(2)
C(4A)-H(4AC)	0.90(3)	S(B)-C(8B)	1.779(3)
C(5A)-H(5AA)	1.01(4)	S(B)-C(7B)	1.781(3)
C(5A)-H(5AB)	1.00(3)	C(7B)-H(7BA)	0.97(3)
C(5A)-H(5AC)	0.85(3)	C(7B)-H(7BB)	0.90(4)
C(6A)-H(6AA)	1.00(4)	C(7B)-H(7BC)	1.00(4)
C(6A)-H(6AB)	0.91(4)	C(8B)-H(8BA)	0.96(3)
C(6A)-H(6AC)	1.02(4)	C(8B)-H(8BB)	0.94(4)
S(A)-O(A)	1.476(2)	C(8B)-H(8BC)	0.96(3)
S(A)-C(8A)	1.781(3)		
S(A)-C(7A)	1.783(3)	N(2A)-Ru(A)-N(1A)	82.72(9)
C(7A)-H(7AA)	1.07(4)	N(2A)-Ru(A)-S(A)	96.02(6)
C(7A)-H(7AB)	0.93(3)	N(1A)-Ru(A)-S(A)	176.77(6)
C(7A)-H(7AC)	0.95(4)	N(2A)-Ru(A)-Cl(3A)	88.17(6)
C(8A)-H(8AA)	1.06(4)	N(1A)-Ru(A)-Cl(3A)	91.74(6)
C(8A)-H(8AB)	1.00(3)	S(A)-Ru(A)-Cl(3A)	91.20(3)
C(8A)-H(8AC)	0.94(4)	N(2A)-Ru(A)-Cl(1A)	91.87(6)
Ru(B)-N(1B)	2.190(2)	N(1A)-Ru(A)-Cl(1A)	89.95(6)
Ru(B)-N(2B)	2.198(2)	S(A)-Ru(A)-Cl(1A)	87.11(3)
Ru(B)-S(B)	2.2912(9)	Cl(3A)-Ru(A)-Cl(1A)	178.31(2)
Ru(B)-Cl(3B)	2.3327(7)	N(2A)-Ru(A)-Cl(2A)	173.38(6)
Ru(B)-Cl(2B)	2.3457(8)	N(1A)-Ru(A)-Cl(2A)	91.62(7)
Ru(B)-Cl(1B)	2.3466(8)	S(A)-Ru(A)-Cl(2A)	89.81(3)
N(1B)-C(3B)	1.458(5)	Cl(3A)-Ru(A)-Cl(2A)	88.57(2)
N(1B)-C(4B)	1.477(7)	Cl(1A)-Ru(A)-Cl(2A)	91.55(2)
N(1B)-C(1B2)	1.490(7)	C(1A)-N(1A)-C(4A)	110.9(2)
N(1B)-C(1B1)	1.607(6)	C(1A)-N(1A)-C(3A)	108.9(2)
N(2B)-C(5B)	1.483(4)	C(4A)-N(1A)-C(3A)	105.1(2)
N(2B)-C(2B)	1.487(4)	C(1A)-N(1A)-Ru(A)	104.41(17)
N(2B)-C(6B)	1.494(5)	C(4A)-N(1A)-Ru(A)	114.57(18)

C(3A)-N(1A)-Ru(A)	112.94(18)
C(5A)-N(2A)-C(6A)	105.4(2)
C(5A)-N(2A)-C(2A)	109.7(2)
C(6A)-N(2A)-C(2A)	107.7(2)
C(5A)-N(2A)-Ru(A)	114.45(18)
C(6A)-N(2A)-Ru(A)	115.42(18)
C(2A)-N(2A)-Ru(A)	103.99(16)
N(1A)-C(1A)-C(2A)	109.8(3)
N(1A)-C(1A)-H(1AA)	109(2)
C(2A)-C(1A)-H(1AA)	111(2)
N(1A)-C(1A)-H(1AB)	108(2)
C(2A)-C(1A)-H(1AB)	109(2)
H(1AA)-C(1A)-H(1AB)	111(3)
C(1A)-C(2A)-N(2A)	111.0(2)
C(1A)-C(2A)-H(2AA)	110.9(15)
N(2A)-C(2A)-H(2AA)	102.9(15)
C(1A)-C(2A)-H(2AB)	115(2)
N(2A)-C(2A)-H(2AB)	108(2)
H(2AA)-C(2A)-H(2AB)	108(3)
N(1A)-C(3A)-H(3AA)	102.9(19)
N(1A)-C(3A)-H(3AB)	111.7(19)
H(3AA)-C(3A)-H(3AB)	113(3)
N(1A)-C(3A)-H(3AC)	112(2)
H(3AA)-C(3A)-H(3AC)	104(3)
H(3AB)-C(3A)-H(3AC)	112(3)
N(1A)-C(4A)-H(4AA)	112(2)
N(1A)-C(4A)-H(4AB)	113.4(18)
H(4AA)-C(4A)-H(4AB)	107(3)
N(1A)-C(4A)-H(4AC)	109(2)
H(4AA)-C(4A)-H(4AC)	106(3)
H(4AB)-C(4A)-H(4AC)	108(3)
N(2A)-C(5A)-H(5AA)	113(2)
N(2A)-C(5A)-H(5AB)	113.9(19)
H(5AA)-C(5A)-H(5AB)	105(3)
N(2A)-C(5A)-H(5AC)	108(2)
H(5AA)-C(5A)-H(5AC)	107(3)
H(5AB)-C(5A)-H(5AC)	111(3)
N(2A)-C(6A)-H(6AA)	111(2)
N(2A)-C(6A)-H(6AB)	109(2)
H(6AA)-C(6A)-H(6AB)	106(3)
N(2A)-C(6A)-H(6AC)	111(2)
H(6AA)-C(6A)-H(6AC)	107(3)
H(6AB)-C(6A)-H(6AC)	113(3)
O(A)-S(A)-C(8A)	108.82(17)
O(A)-S(A)-C(7A)	106.98(16)
C(8A)-S(A)-C(7A)	99.08(16)
O(A)-S(A)-Ru(A)	116.51(10)
C(8A)-S(A)-Ru(A)	112.61(12)
C(7A)-S(A)-Ru(A)	111.31(12)
S(A)-C(7A)-H(7AA)	104(2)
S(A)-C(7A)-H(7AB)	103(2)
H(7AA)-C(7A)-H(7AB)	115(3)
S(A)-C(7A)-H(7AC)	109(2)
H(7AA)-C(7A)-H(7AC)	110(3)
H(7AB)-C(7A)-H(7AC)	115(3)
S(A)-C(8A)-H(8AA)	112(2)
S(A)-C(8A)-H(8AB)	105.6(18)
H(8AA)-C(8A)-H(8AB)	109(3)
S(A)-C(8A)-H(8AC)	107(2)
H(8AA)-C(8A)-H(8AC)	114(3)
H(8AB)-C(8A)-H(8AC)	109(3)
N(1B)-Ru(B)-N(2B)	82.96(10)
N(1B)-Ru(B)-S(B)	179.84(9)
N(2B)-Ru(B)-S(B)	96.98(7)
N(1B)-Ru(B)-Cl(3B)	91.04(9)
N(2B)-Ru(B)-Cl(3B)	89.17(7)
S(B)-Ru(B)-Cl(3B)	88.82(3)
N(1B)-Ru(B)-Cl(2B)	90.81(7)
N(2B)-Ru(B)-Cl(2B)	173.77(7)
S(B)-Ru(B)-Cl(2B)	89.25(3)
Cl(3B)-Ru(B)-Cl(2B)	90.86(3)
N(1B)-Ru(B)-Cl(1B)	90.96(9)
N(2B)-Ru(B)-Cl(1B)	89.55(7)
S(B)-Ru(B)-Cl(1B)	89.18(3)
Cl(3B)-Ru(B)-Cl(1B)	177.48(3)
Cl(2B)-Ru(B)-Cl(1B)	90.65(3)
C(3B)-N(1B)-C(4B)	104.7(3)
C(3B)-N(1B)-C(1B2)	125.9(4)
C(4B)-N(1B)-C(1B2)	86.8(4)
C(3B)-N(1B)-C(1B1)	97.0(3)
C(4B)-N(1B)-C(1B1)	125.5(4)
C(1B2)-N(1B)-C(1B1)	41.6(3)
C(3B)-N(1B)-Ru(B)	115.1(2)
C(4B)-N(1B)-Ru(B)	114.1(3)
C(1B2)-N(1B)-Ru(B)	106.8(3)
C(1B1)-N(1B)-Ru(B)	99.9(2)
C(5B)-N(2B)-C(2B)	108.2(3)
C(5B)-N(2B)-C(6B)	105.3(3)
C(2B)-N(2B)-C(6B)	110.1(4)
C(5B)-N(2B)-Ru(B)	114.79(18)
C(2B)-N(2B)-Ru(B)	103.7(2)
C(6B)-N(2B)-Ru(B)	114.7(2)
C(2B)-C(1B1)-N(1B)	112.6(4)
C(2B)-C(1B1)-H(1BA)	109.1
N(1B)-C(1B1)-H(1BA)	109.1
C(2B)-C(1B1)-H(1BB)	109.1
N(1B)-C(1B1)-H(1BB)	109.1
H(1BA)-C(1B1)-H(1BB)	107.8
C(2B)-C(1B2)-N(1B)	109.3(5)
C(2B)-C(1B2)-C(4B)	147.0(5)
N(1B)-C(1B2)-C(4B)	46.3(2)
C(2B)-C(1B2)-H(1BC)	109.8
N(1B)-C(1B2)-H(1BC)	109.8
C(4B)-C(1B2)-H(1BC)	70.3
C(2B)-C(1B2)-H(1BD)	109.8
N(1B)-C(1B2)-H(1BD)	109.8
C(4B)-C(1B2)-H(1BD)	100.8
H(1BC)-C(1B2)-H(1BD)	108.3

C(1B1)-C(2B)-C(1B2)	47.6(4)
C(1B1)-C(2B)-N(2B)	118.4(4)
C(1B2)-C(2B)-N(2B)	121.8(4)
C(1B1)-C(2B)-H(2BA)	107.7
C(1B2)-C(2B)-H(2BA)	130.5
N(2B)-C(2B)-H(2BA)	107.7
C(1B1)-C(2B)-H(2BB)	107.7
C(1B2)-C(2B)-H(2BB)	61.5
N(2B)-C(2B)-H(2BB)	107.7
H(2BA)-C(2B)-H(2BB)	107.1
N(1B)-C(3B)-H(3BA)	113(2)
N(1B)-C(3B)-H(3BB)	110(2)
H(3BA)-C(3B)-H(3BB)	103(3)
N(1B)-C(3B)-H(3BC)	116(3)
H(3BA)-C(3B)-H(3BC)	105(3)
H(3BB)-C(3B)-H(3BC)	108(3)
N(1B)-C(4B)-C(1B2)	46.8(3)
N(1B)-C(4B)-H(4BA)	110(3)
C(1B2)-C(4B)-H(4BA)	93(3)
N(1B)-C(4B)-H(4BB)	102(6)
C(1B2)-C(4B)-H(4BB)	64(6)
H(4BA)-C(4B)-H(4BB)	104(6)
N(1B)-C(4B)-H(4BC)	105(5)
C(1B2)-C(4B)-H(4BC)	151(5)
H(4BA)-C(4B)-H(4BC)	108(6)
H(4BB)-C(4B)-H(4BC)	126(8)
N(2B)-C(5B)-H(5BA)	109(2)
N(2B)-C(5B)-H(5BB)	110(2)
H(5BA)-C(5B)-H(5BB)	109(3)
N(2B)-C(5B)-H(5BC)	112(2)
H(5BA)-C(5B)-H(5BC)	110(3)
H(5BB)-C(5B)-H(5BC)	108(3)
N(2B)-C(6B)-H(6BA)	106(2)
N(2B)-C(6B)-H(6BB)	117(3)
H(6BA)-C(6B)-H(6BB)	99(4)
N(2B)-C(6B)-H(6BC)	108(2)
H(6BA)-C(6B)-H(6BC)	106(3)
H(6BB)-C(6B)-H(6BC)	119(4)
O(B)-S(B)-C(8B)	107.72(14)
O(B)-S(B)-C(7B)	107.60(15)
C(8B)-S(B)-C(7B)	98.79(17)
O(B)-S(B)-Ru(B)	117.71(9)
C(8B)-S(B)-Ru(B)	111.20(11)
C(7B)-S(B)-Ru(B)	112.07(11)
S(B)-C(7B)-H(7BA)	108.5(19)
S(B)-C(7B)-H(7BB)	109(2)
H(7BA)-C(7B)-H(7BB)	109(3)
S(B)-C(7B)-H(7BC)	109(2)
H(7BA)-C(7B)-H(7BC)	110(3)
H(7BB)-C(7B)-H(7BC)	111(3)
S(B)-C(8B)-H(8BA)	104.9(17)
S(B)-C(8B)-H(8BB)	108(2)
H(8BA)-C(8B)-H(8BB)	113(3)
S(B)-C(8B)-H(8BC)	108(2)
H(8BA)-C(8B)-H(8BC)	111(3)
H(8BB)-C(8B)-H(8BC)	111(3)

Table 4. Anisotropic displacement parameters ($Å^2 x 10^3$) for JJR2 $RuCl_3(DMSO)(TMEDA)$. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ru(A)	9(1)	9(1)	9(1)	1(1)	1(1)	-1(1)
Cl(1A)	12(1)	21(1)	17(1)	0(1)	-2(1)	-4(1)
Cl(2A)	20(1)	13(1)	30(1)	7(1)	-1(1)	-3(1)
Cl(3A)	14(1)	22(1)	18(1)	1(1)	-4(1)	-1(1)
N(1A)	13(1)	29(1)	12(1)	-6(1)	6(1)	-4(1)
N(2A)	18(1)	14(1)	23(1)	2(1)	6(1)	-1(1)
C(1A)	26(2)	26(2)	29(2)	-10(1)	9(1)	-2(1)
C(2A)	28(2)	13(1)	36(2)	0(1)	10(1)	4(1)
C(3A)	26(2)	45(2)	12(1)	0(1)	4(1)	-2(1)
C(4A)	19(1)	34(2)	24(2)	0(1)	11(1)	-4(1)
C(5A)	19(2)	17(2)	46(2)	5(1)	9(2)	-6(1)
C(6A)	33(2)	25(2)	28(2)	15(1)	2(1)	5(1)
S(A)	20(1)	21(1)	15(1)	-2(1)	5(1)	4(1)
O(A)	52(2)	37(1)	34(1)	5(1)	26(1)	2(1)
C(7A)	20(2)	34(2)	27(2)	-8(1)	0(1)	11(1)
C(8A)	29(2)	41(2)	23(2)	-16(2)	-6(1)	10(2)
Ru(B)	13(1)	8(1)	10(1)	-1(1)	4(1)	-1(1)
Cl(1B)	64(1)	19(1)	12(1)	-3(1)	14(1)	-6(1)
Cl(2B)	20(1)	13(1)	28(1)	0(1)	6(1)	4(1)
Cl(3B)	26(1)	24(1)	11(1)	2(1)	0(1)	-2(1)
N(1B)	19(1)	22(1)	74(2)	-16(1)	25(1)	-9(1)
N(2B)	27(1)	10(1)	25(1)	0(1)	-4(1)	-1(1)
C(2B)	41(2)	11(2)	184(6)	17(2)	-51(3)	-15(2)
C(3B)	18(2)	64(3)	42(2)	29(2)	17(2)	9(2)
C(4B)	17(2)	211(9)	59(3)	-90(5)	16(2)	-44(3)
C(5B)	28(2)	23(2)	24(2)	9(1)	6(1)	10(1)
C(6B)	100(4)	34(2)	21(2)	-7(2)	1(2)	42(2)
S(B)	13(1)	14(1)	17(1)	-2(1)	1(1)	-2(1)
O(B)	20(1)	31(1)	35(1)	-1(1)	3(1)	5(1)
C(7B)	22(2)	29(2)	28(2)	-15(1)	-2(1)	-6(1)
C(8B)	22(2)	19(1)	34(2)	5(1)	9(1)	-7(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for JJR2 $RuCl_3$(DMSO)(TMEDA).

	x	y	z	U(eq)
H(1AA)	1940(20)	7750(40)	2191(13)	25(9)
H(1AB)	860(30)	8100(40)	2304(16)	55(12)
H(2AA)	340(20)	7940(30)	1307(12)	18(8)
H(2AB)	1130(30)	9270(40)	1470(15)	42(11)
H(3AA)	1280(20)	5830(40)	2852(14)	26(9)
H(3AB)	1390(20)	4030(40)	2593(14)	37(10)
H(3AC)	2230(30)	5440(40)	2643(15)	39(10)
H(4AA)	-210(20)	6020(40)	2384(15)	45(11)
H(4AB)	-340(20)	6140(30)	1718(13)	21(8)
H(4AC)	-50(20)	4640(40)	2013(13)	24(9)
H(5AA)	2610(20)	9420(40)	1076(14)	35(10)
H(5AB)	2990(20)	8220(40)	1548(14)	31(9)
H(5AC)	2980(20)	7870(40)	933(14)	28(10)
H(6AA)	1220(20)	9050(40)	464(14)	40(10)
H(6AB)	1630(30)	7540(40)	285(15)	39(11)
H(6AC)	570(30)	7520(40)	451(15)	47(11)
H(7AA)	3520(30)	2460(50)	397(18)	75(14)
H(7AB)	3810(20)	3450(40)	985(14)	28(9)
H(7AC)	3070(20)	2090(40)	974(15)	36(10)
H(8AA)	2030(30)	2610(40)	-195(16)	58(12)
H(8AB)	1400(20)	2330(40)	336(13)	24(9)
H(8AC)	1150(30)	3780(40)	-38(15)	42(11)
H(1BA)[a]	8700	3500	1165	34(16)
H(1BB)[a]	7963	2767	685	18(13)
H(1BC)[b]	8382	2671	1945	16(19)
H(1BD)[b]	8885	3343	1442	30(20)
H(2BA)	7305	4401	1140	101
H(2BB)	7667	3545	1703	101
H(3BA)	9550(30)	1140(40)	897(15)	40(11)
H(3BB)	9130(20)	-410(40)	901(15)	32(10)
H(3BC)	8690(30)	880(50)	525(18)	66(14)
H(4BA)	9710(40)	1260(60)	1820(20)	113
H(4BB)	8880(40)	1170(70)	2010(30)	113
H(4BC)	9120(50)	-60(70)	1830(30)	113
H(5BA)	5760(20)	4000(40)	788(13)	22(8)
H(5BB)	6300(30)	2890(40)	435(16)	49(11)
H(5BC)	5380(20)	2380(40)	682(14)	35(10)
H(6BA)	5830(20)	4080(40)	1670(14)	36(10)
H(6BB)	5360(40)	2560(60)	1710(20)	100(20)
H(6BC)	6400(30)	2870(40)	2054(16)	41(11)
H(7BA)	4670(20)	-2790(40)	700(13)	26(9)
H(7BB)	5170(20)	-1680(40)	350(15)	35(10)
H(7BC)	5800(30)	-2980(40)	659(15)	45(11)
H(8BA)	4860(20)	-2880(30)	1681(12)	16(8)
H(8BB)	6000(30)	-2990(40)	1786(14)	40(10)
H(8BC)	5460(20)	-1790(40)	2116(14)	34(10)

[a] Population 0.59(1)
[b] Population 0.41(1)

Figure 1. Structure of the non-disordered molecule of *mer*-[$RuCl_3$(dmso)(tmen)] (View A).

Figure 2. Structure of the non-disordered molecule of *mer*-[$RuCl_3$(dmso)(tmen)]. View looks down the N1–Ru–S axis (View B).

Figure 3. Structure of the disordered molecule of *mer*-[$RuCl_3$(dmso)(tmen)] (View A)

Figure 4. Structure of the disordered molecule of *mer*-[$RuCl_3$(dmso)(tmen)] (View B).

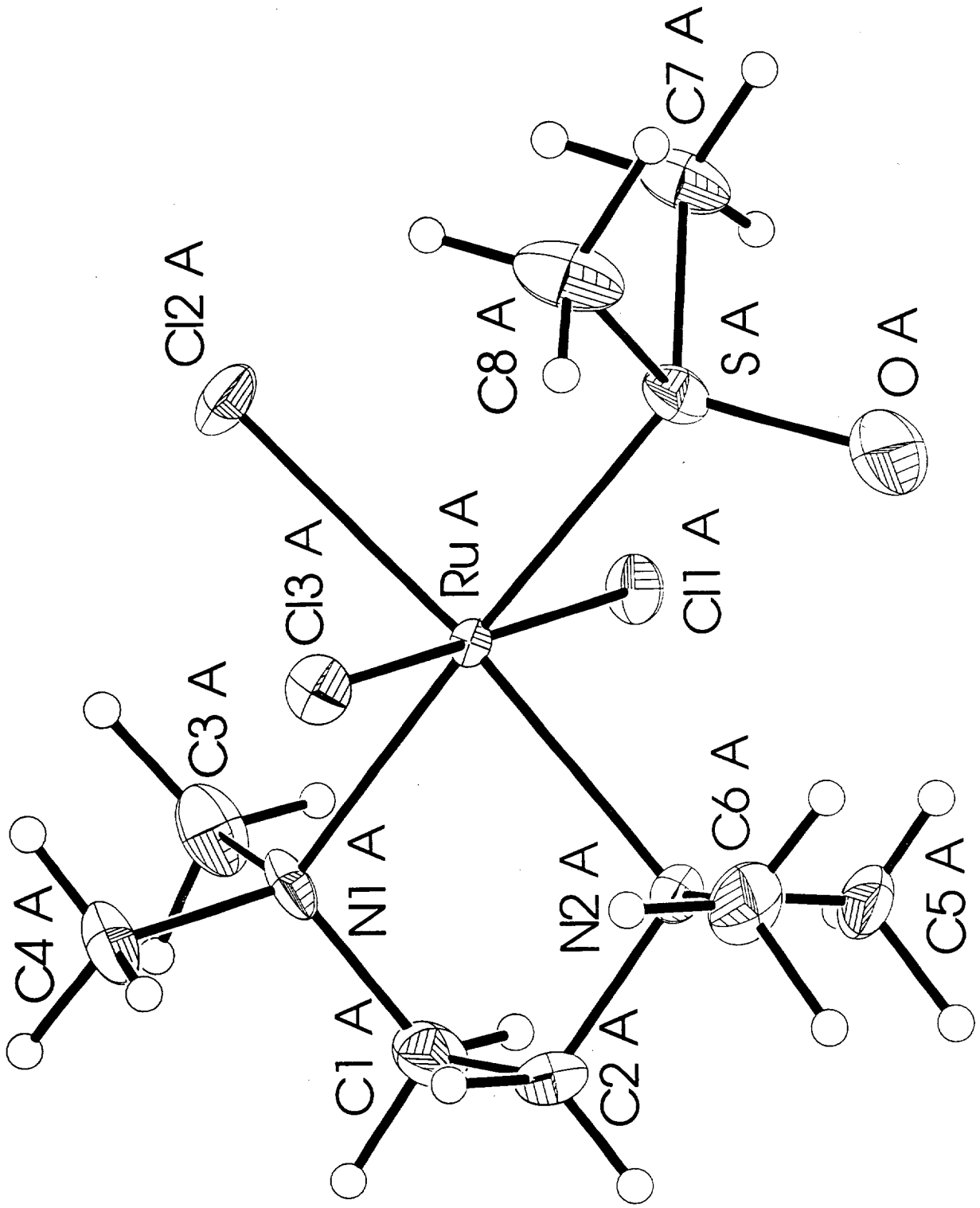
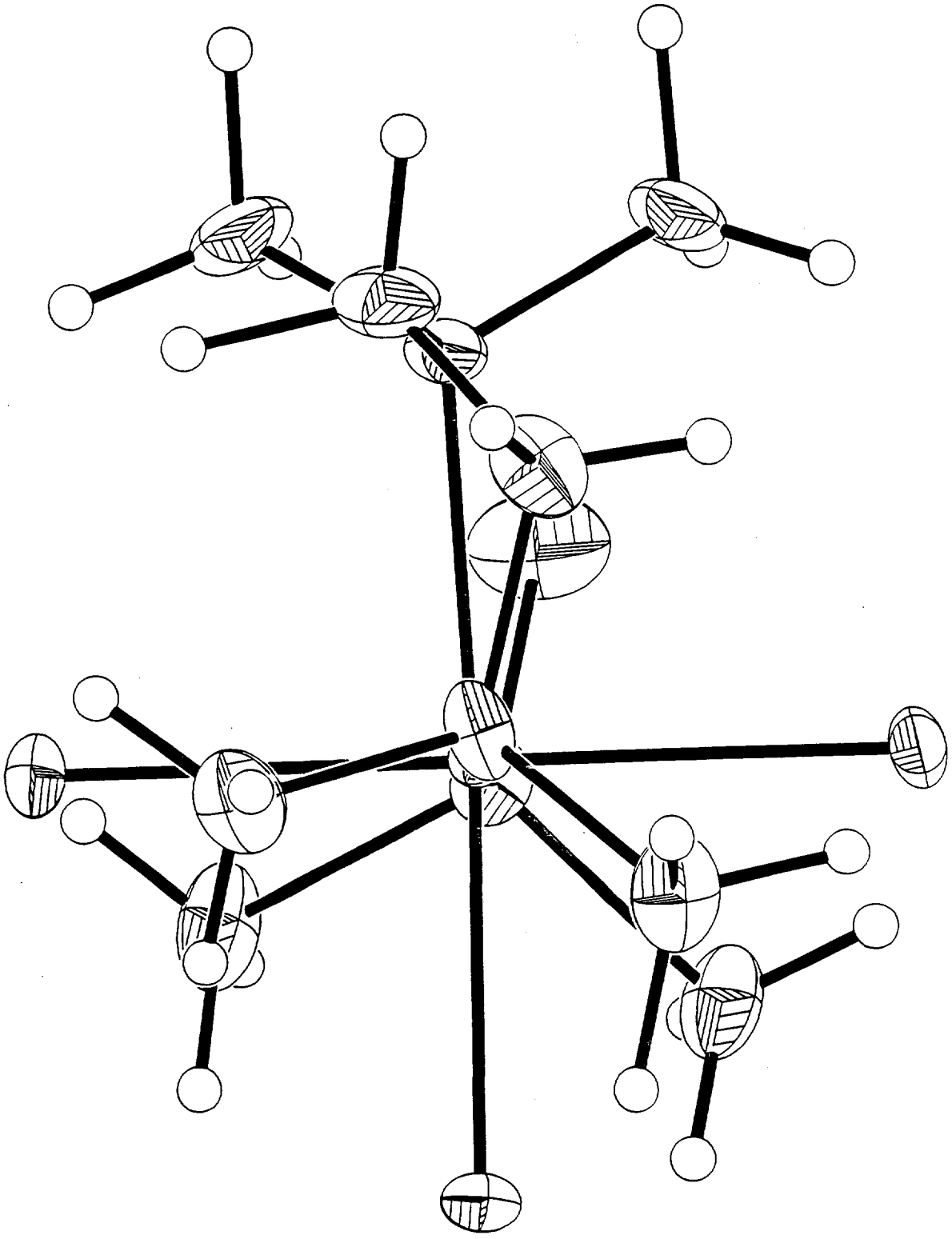


Fig. S1

Fig S2



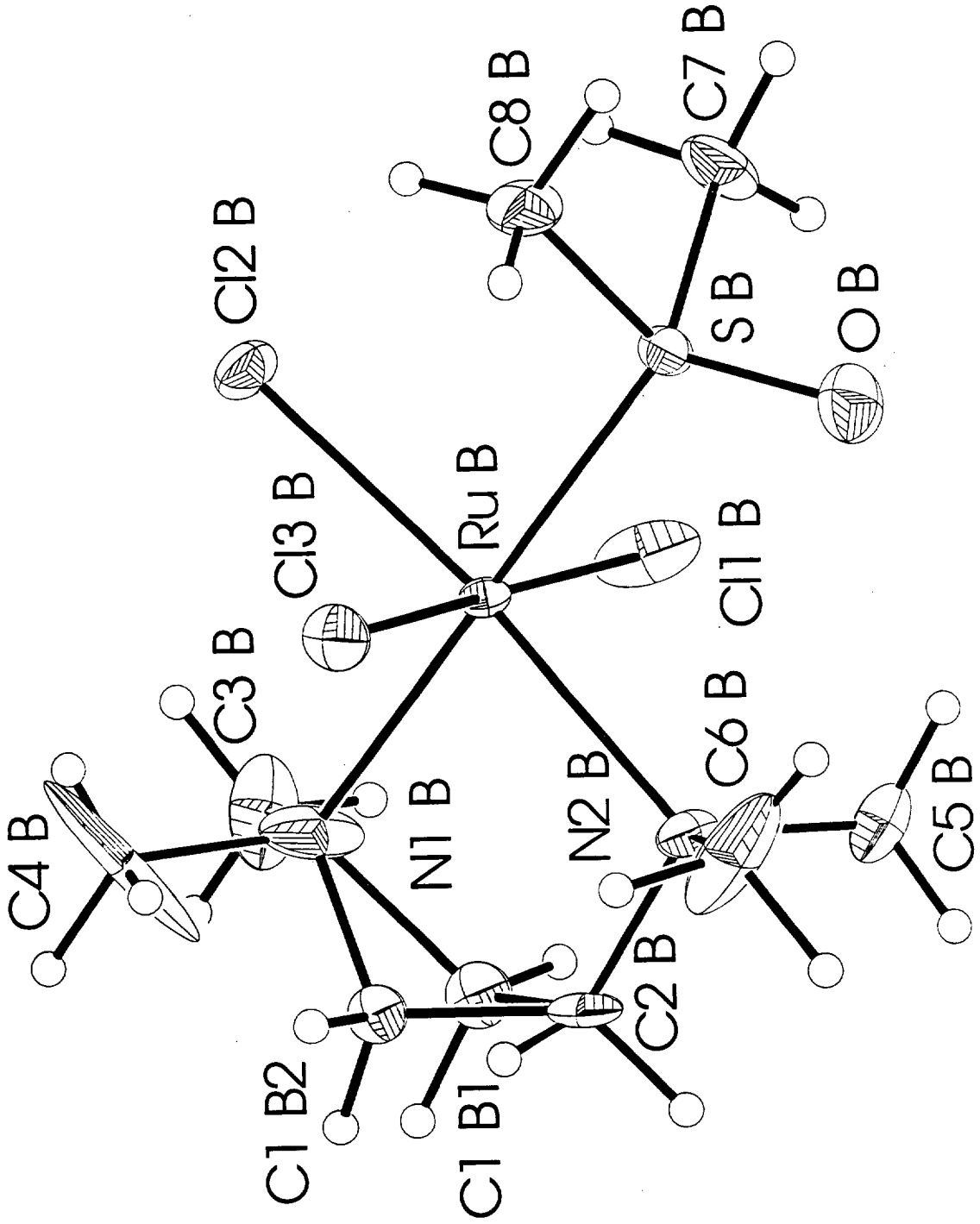


Fig S3

Fig. S4