FIVE-MEMBERED SULFUR-NITROGEN RING COMPOUNDS

Supplementary material

Vit Matuska

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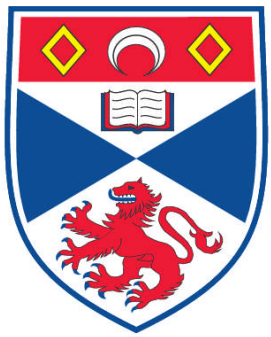

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Five-Membered Sulfur-Nitrogen Ring Compounds

Supplementary Material

To the thesis submitted by

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Table 1.1 Crystal data and structure refinement for $PhAs(S_2N_2)$ (**34**)

Identification code	vmdw24	
Empirical formula	C6 H5 As N2 S2	
Formula weight	244.16	
Temperature	93(2) K	
Wavelength	0.710 73 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 5.046(2) Å	α = 103.427(13)°
	b = 8.330(4) Å	β = 91.802(15)°
	c = 10.155(6) Å	γ = 93.833(13)°
Volume	413.8(4) Å^3	
Z	2	
Density (calculated)	1.960 Mg/m^3	
Absorption coefficient	4.541 mm^{-1}	
F(000)	240	
Crystal size	0.2000 × 0.0500 × 0.0300 mm^3	
Theta range for data collection	2.06 to 25.34°.	
Index ranges	$-6 \leq h \leq 5, -10 \leq k \leq 8, -9 \leq l \leq 12$	
Reflections collected	2456	
Independent reflections	1367 [R(int) = 0.0313]	
Completeness to theta = 25.00°	91.5 %	
Absorption correction	Multiscan	
Max. and min. transmission	1.0000 and 0.6345	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1367 / 0 / 101	
Goodness-of-fit on F^2	1.118	
Final R indices [I>2sigma(I)]	R1 = 0.0477, wR2 = 0.1047	
R indices (all data)	R1 = 0.0546, wR2 = 0.1114	
Largest diff. peak and hole	0.883 and −1.042 e·Å^{-3}	

Table 1.2 Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for $PhAs(S_2N_2)$ (**34**). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
As(1)	9746(1)	2492(1)	1434(1)	24(1)
N(1)	7576(10)	3839(6)	655(5)	22(1)
S(1)	7408(3)	5632(2)	1473(2)	27(1)
N(2)	9325(9)	6172(6)	2776(5)	22(1)
S(2)	11353(3)	4779(2)	3078(2)	27(1)
C(1)	6923(12)	1561(7)	2389(6)	22(1)
C(2)	5958(12)	2418(7)	3613(6)	23(1)
C(3)	3854(12)	1683(8)	4178(6)	25(1)
C(4)	2740(13)	112(8)	3536(6)	28(1)
C(5)	3708(12)	-729(7)	2338(6)	26(1)
C(6)	5802(13)	-17(7)	1761(6)	25(1)

Table 1.3 Bond lengths [Å] and angles [°] for $PhAs(S_2N_2)$ (**34**)

As(1)−N(1)	1.899(5)
As(1)−C(1)	1.965(6)
As(1)−S(2)	2.3028(19)
N(1)−S(1)	1.540(5)
S(1)−N(2)	1.573(5)
N(2)−S(2)	1.671(5)
C(1)−C(6)	1.394(8)
C(1)−C(2)	1.402(8)
C(2)−C(3)	1.395(8)
C(2)−H(2A)	0.9500
C(3)−C(4)	1.391(9)
C(3)−H(3A)	0.9500
C(4)−C(5)	1.377(9)
C(4)−H(4A)	0.9500
C(5)−C(6)	1.389(9)
C(5)−H(5A)	0.9500
C(6)−H(6A)	0.9500
N(1)−As(1)−C(1)	96.5(2)
N(1)−As(1)−S(2)	90.01(15)
C(1)−As(1)−S(2)	101.07(17)
S(1)−N(1)−As(1)	116.6(3)
N(1)−S(1)−N(2)	115.1(3)
S(1)−N(2)−S(2)	116.9(3)
N(2)−S(2)−As(1)	100.23(18)
C(6)−C(1)−C(2)	119.9(5)
C(6)−C(1)−As(1)	116.5(4)
C(2)−C(1)−As(1)	123.6(4)
C(3)−C(2)−C(1)	119.2(5)
C(3)−C(2)−H(2A)	120.4
C(1)−C(2)−H(2A)	120.4
C(4)−C(3)−C(2)	120.3(5)
C(4)−C(3)−H(3A)	119.9
C(2)−C(3)−H(3A)	119.9
C(5)−C(4)−C(3)	120.2(6)
C(5)−C(4)−H(4A)	119.9
C(3)−C(4)−H(4A)	119.9
C(4)−C(5)−C(6)	120.3(6)
C(4)−C(5)−H(5A)	119.8
C(6)−C(5)−H(5A)	119.8
C(5)−C(6)−C(1)	120.0(6)
C(5)−C(6)−H(6A)	120.0
C(1)−C(6)−H(6A)	120.0

Symmetry transformations used to generate equivalent atoms:

Table 1.4 Anisotropic displacement parameters ($Å^2 \times 10^3$) for $PhAs(S_2N_2)$ (**34**). The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2\ a^{*2}\ U^{11} + \ldots + 2\ h\ k\ a^*\ b^*\ U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
As(1)	24(1)	18(1)	29(1)	3(1)	8(1)	2(1)
N(1)	24(3)	19(3)	21(3)	0(2)	6(2)	-2(2)
S(1)	30(1)	20(1)	31(1)	7(1)	5(1)	3(1)
N(2)	18(3)	18(3)	26(3)	-3(2)	2(2)	-3(2)
S(2)	24(1)	22(1)	31(1)	3(1)	1(1)	-2(1)
C(1)	24(3)	14(3)	26(3)	3(2)	-2(3)	2(2)
C(2)	30(4)	14(3)	21(3)	-1(2)	-1(2)	0(2)
C(3)	29(4)	23(3)	23(3)	3(2)	2(3)	5(3)
C(4)	29(4)	28(4)	29(3)	10(3)	7(3)	6(3)
C(5)	31(4)	14(3)	33(3)	6(3)	0(3)	-2(3)
C(6)	31(4)	21(3)	22(3)	1(2)	0(3)	6(3)

Table 1.5 Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($Å^2 \times 10^3$) for $PhAs(S_2N_2)$ (**34**)

	x	y	z	U(eq)
H(2A)	6729	3488	4054	27
H(3A)	3179	2257	5004	30
H(4A)	1307	-382	3925	33
H(5A)	2940	-1801	1904	31
H(6A)	6471	-605	937	30

Table 1.6 Torsion angles [°] for $PhAs(S_2N_2)$ (**34**)

C(1)−As(1)−N(1)−S(1)	91.9(3)
S(2)−As(1)−N(1)−S(1)	−9.3(3)
As(1)−N(1)−S(1)−N(2)	6.6(4)
N(1)−S(1)−N(2)−S(2)	2.1(4)
S(1)−N(2)−S(2)−As(1)	−7.7(3)
N(1)−As(1)−S(2)−N(2)	9.0(2)
C(1)−As(1)−S(2)−N(2)	−87.6(2)
N(1)−As(1)−C(1)−C(6)	99.3(5)
S(2)−As(1)−C(1)−C(6)	−169.4(4)
N(1)−As(1)−C(1)−C(2)	−78.4(5)
S(2)−As(1)−C(1)−C(2)	12.9(5)
C(6)−C(1)−C(2)−C(3)	−0.9(9)
As(1)−C(1)−C(2)−C(3)	176.7(4)
C(1)−C(2)−C(3)−C(4)	0.4(9)
C(2)−C(3)−C(4)−C(5)	0.0(9)
C(3)−C(4)−C(5)−C(6)	0.0(9)
C(4)−C(5)−C(6)−C(1)	−0.4(9)
C(2)−C(1)−C(6)−C(5)	0.9(9)
As(1)−C(1)−C(6)−C(5)	−176.9(4)

Symmetry transformations used to generate equivalent atoms:

2 Full X-ray data of MesAs(S_2N_2)

Table 2.1 Crystal data and structure refinement for MesAs(S_2N_2) (**35**)

Identification code	vmdw42	
Empirical formula	C9 H11 As N2 S2	
Formula weight	286.24	
Temperature	93(2) K	
Wavelength	0.710 73 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 14.367(6) Å	$\alpha = 90°$
	b = 11.372(5) Å	$\beta = 91.685(10)°$
	c = 13.911(5) Å	$\gamma = 90°$
Volume	2271.8(16) $Å^3$	
Z	8	
Density (calculated)	1.674 Mg/m^3	
Absorption coefficient	3.322 mm^{-1}	
F(000)	1152	
Crystal size	0.1000 × 0.0300 × 0.0300 mm^3	
Theta range for data collection	1.42 to 25.35°.	
Index ranges	$-17 \leq h \leq 13, -13 \leq k \leq 12, -15 \leq l \leq 16$	
Reflections collected	14163	
Independent reflections	4133 [R(int) = 0.1453]	
Completeness to theta = 25.00°	99.4 %	
Absorption correction	Multiscan	
Max. and min. transmission	1.0000 and 0.9268	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4133 / 0 / 261	
Goodness-of-fit on F^2	1.028	
Final R indices [I>2sigma(I)]	R1 = 0.0901, wR2 = 0.2210	
R indices (all data)	R1 = 0.1388, wR2 = 0.2572	
Extinction coefficient	0.0056(12)	
Largest diff. peak and hole	0.854 and −0.750 e·$Å^{-3}$	

Table 2.2 Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for MesAs(S_2N_2) (**35**). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
As(1)	2570(1)	845(1)	1439(1)	67(1)
N(1)	1903(5)	1657(7)	2420(5)	70(2)
S(1)	1300(2)	2695(3)	2052(2)	94(1)
N(2)	1290(5)	2954(7)	948(5)	65(2)
S(2)	1973(2)	2123(3)	281(2)	81(1)
C(1)	1859(6)	-622(9)	1257(5)	61(3)
C(2)	885(6)	-763(9)	1194(5)	60(2)
C(3)	518(6)	-1889(10)	1071(5)	72(3)
C(4)	1067(7)	-2848(9)	1010(5)	63(2)
C(5)	2003(6)	-2735(10)	1057(5)	66(3)
C(6)	2423(6)	-1629(10)	1174(5)	61(3)
C(7)	221(6)	258(10)	1250(6)	75(3)
C(8)	598(8)	-4063(10)	903(7)	94(4)
C(9)	3493(5)	-1583(9)	1234(5)	70(3)
As(11)	2506(1)	5628(1)	3411(1)	71(1)
N(11)	3185(5)	4649(7)	4271(5)	72(2)
S(11)	3928(2)	3829(3)	3865(2)	87(1)
N(12)	4007(6)	3873(8)	2752(5)	84(2)
S(12)	3294(2)	4772(3)	2141(2)	90(1)
C(11)	3064(5)	7193(9)	3634(5)	60(2)
C(12)	4010(6)	7451(10)	3735(5)	65(3)
C(13)	4276(6)	8623(11)	3894(5)	72(3)
C(14)	3625(7)	9510(10)	3935(6)	72(3)
C(15)	2691(6)	9223(10)	3835(5)	67(3)
C(16)	2393(5)	8092(10)	3683(5)	63(3)
C(17)	4788(6)	6561(9)	3665(7)	73(3)
C(18)	3939(8)	10774(10)	4081(7)	95(4)
C(19)	1362(5)	7880(9)	3574(5)	64(2)

Table 2.3 Bond lengths [Å] and angles [°] for MesAs(S_2N_2) (**35**)

As(1)−N(1)	1.927(7)
As(1)−C(1)	1.969(9)
As(1)−S(2)	2.315(3)
N(1)−S(1)	1.543(8)
S(1)−N(2)	1.563(7)
N(2)−S(2)	1.665(7)
C(1)−C(6)	1.409(12)
C(1)−C(2)	1.410(11)
C(2)−C(3)	1.393(13)
C(2)−C(7)	1.505(13)
C(3)−C(4)	1.350(13)
C(3)−H(3A)	0.9500
C(4)−C(5)	1.350(12)
C(4)−C(8)	1.542(13)
C(5)−C(6)	1.402(13)
C(5)−H(5A)	0.9500
C(6)−C(9)	1.537(11)
C(7)−H(7A)	0.9800
C(7)−H(7B)	0.9800
C(7)−H(7C)	0.9800
C(8)−H(8A)	0.9800
C(8)−H(8B)	0.9800
C(8)−H(8C)	0.9800
C(9)−H(9A)	0.9800
C(9)−H(9B)	0.9800
C(9)−H(9C)	0.9800
As(11)−N(11)	1.886(7)
As(11)−C(11)	1.973(9)
As(11)−S(12)	2.339(3)
N(11)−S(11)	1.537(7)
S(11)−N(12)	1.556(8)
N(12)−S(12)	1.663(9)
C(11)−C(12)	1.393(11)
C(11)−C(16)	1.410(12)
C(12)−C(13)	1.402(14)
C(12)−C(17)	1.513(12)
C(13)−C(14)	1.378(13)
C(13)−H(13A)	0.9500
C(14)−C(15)	1.385(13)
C(14)−C(18)	1.518(14)
C(15)−C(16)	1.369(13)
C(15)−H(15A)	0.9500
C(16)−C(19)	1.504(11)
C(17)−H(17A)	0.9800

Table 2.3 continued

C(17)−H(17B)	0.9800
C(17)−H(17C)	0.9800
C(18)−H(18A)	0.9800
C(18)−H(18B)	0.9800
C(18)−H(18C)	0.9800
C(19)−H(19A)	0.9800
C(19)−H(19B)	0.9800
C(19)−H(19C)	0.9800
N(1)−As(1)−C(1)	103.3(3)
N(1)−As(1)−S(2)	90.6(2)
C(1)−As(1)−S(2)	105.2(3)
S(1)−N(1)−As(1)	114.7(4)
N(1)−S(1)−N(2)	117.3(4)
S(1)−N(2)−S(2)	116.9(5)
N(2)−S(2)−As(1)	100.4(3)
C(6)−C(1)−C(2)	118.4(8)
C(6)−C(1)−As(1)	113.7(6)
C(2)−C(1)−As(1)	127.9(8)
C(3)−C(2)−C(1)	118.9(9)
C(3)−C(2)−C(7)	118.5(8)
C(1)−C(2)−C(7)	122.6(9)
C(4)−C(3)−C(2)	122.0(8)
C(4)−C(3)−H(3A)	119.0
C(2)−C(3)−H(3A)	119.0
C(5)−C(4)−C(3)	120.2(9)
C(5)−C(4)−C(8)	121.4(10)
C(3)−C(4)−C(8)	118.3(9)
C(4)−C(5)−C(6)	121.0(10)
C(4)−C(5)−H(5A)	119.5
C(6)−C(5)−H(5A)	119.5
C(5)−C(6)−C(1)	119.4(8)
C(5)−C(6)−C(9)	117.6(9)
C(1)−C(6)−C(9)	122.9(9)
C(2)−C(7)−H(7A)	109.5
C(2)−C(7)−H(7B)	109.5
H(7A)−C(7)−H(7B)	109.5
C(2)−C(7)−H(7C)	109.5
H(7A)−C(7)−H(7C)	109.5
H(7B)−C(7)−H(7C)	109.5
C(4)−C(8)−H(8A)	109.5
C(4)−C(8)−H(8B)	109.5
H(8A)−C(8)−H(8B)	109.5
C(4)−C(8)−H(8C)	109.5

Table 2.3 continued

H(8A)−C(8)−H(8C)	109.5
H(8B)−C(8)−H(8C)	109.5
C(6)−C(9)−H(9A)	109.5
C(6)−C(9)−H(9B)	109.5
H(9A)−C(9)−H(9B)	109.5
C(6)−C(9)−H(9C)	109.5
H(9A)−C(9)−H(9C)	109.5
H(9B)−C(9)−H(9C)	109.5
N(11)−As(11)−C(11)	103.4(3)
N(11)−As(11)−S(12)	88.9(2)
C(11)−As(11)−S(12)	106.9(2)
S(11)−N(11)−As(11)	118.5(4)
N(11)−S(11)−N(12)	114.7(4)
S(11)−N(12)−S(12)	117.8(5)
N(12)−S(12)−As(11)	100.0(3)
C(12)−C(11)−C(16)	120.6(9)
C(12)−C(11)−As(11)	126.7(7)
C(16)−C(11)−As(11)	112.7(6)
C(11)−C(12)−C(13)	118.5(9)
C(11)−C(12)−C(17)	124.9(10)
C(13)−C(12)−C(17)	116.6(8)
C(14)−C(13)−C(12)	121.3(9)
C(14)−C(13)−H(13A)	119.3
C(12)−C(13)−H(13A)	119.3
C(13)−C(14)−C(15)	118.7(11)
C(13)−C(14)−C(18)	120.0(9)
C(15)−C(14)−C(18)	121.3(10)
C(16)−C(15)−C(14)	122.3(10)
C(16)−C(15)−H(15A)	118.8
C(14)−C(15)−H(15A)	118.8
C(15)−C(16)−C(11)	118.5(8)
C(15)−C(16)−C(19)	118.0(9)
C(11)−C(16)−C(19)	123.5(10)
C(12)−C(17)−H(17A)	109.5
C(12)−C(17)−H(17B)	109.5
H(17A)−C(17)−H(17B)	109.5
C(12)−C(17)−H(17C)	109.5
H(17A)−C(17)−H(17C)	109.5
H(17B)−C(17)−H(17C)	109.5
C(14)−C(18)−H(18A)	109.5
C(14)−C(18)−H(18B)	109.5
H(18A)−C(18)−H(18B)	109.5
C(14)−C(18)−H(18C)	109.5
H(18A)−C(18)−H(18C)	109.5

Table 2.3 continued

H(18B)−C(18)−H(18C)	109.5
C(16)−C(19)−H(19A)	109.5
C(16)−C(19)−H(19B)	109.5
H(19A)−C(19)−H(19B)	109.5
C(16)−C(19)−H(19C)	109.5
H(19A)−C(19)−H(19C)	109.5
H(19B)−C(19)−H(19C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 2.4 Anisotropic displacement parameters (Å$^2\times10^3$) for MesAs(S_2N_2) (**35**). The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2\ a^{*2}\ U^{11} + \ldots + 2\ h\ k\ a^*\ b^*\ U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
As(1)	34(1)	118(1)	49(1)	-7(1)	-2(1)	-15(1)
N(1)	44(4)	102(6)	63(4)	4(4)	-3(3)	-7(4)
S(1)	68(2)	137(3)	76(2)	-24(2)	9(1)	-6(2)
N(2)	48(4)	91(6)	57(4)	-3(4)	0(3)	8(4)
S(2)	57(2)	122(2)	65(1)	1(2)	4(1)	-15(2)
C(1)	39(5)	111(8)	33(4)	-4(4)	2(3)	-26(5)
C(2)	31(4)	118(8)	33(4)	-3(4)	4(3)	-11(5)
C(3)	43(5)	136(10)	36(4)	-2(5)	-4(3)	-34(6)
C(4)	59(6)	91(7)	38(4)	-1(4)	0(4)	-14(6)
C(5)	65(6)	105(8)	28(4)	-4(4)	-2(4)	-4(6)
C(6)	41(5)	113(8)	30(4)	0(5)	6(3)	1(5)
C(7)	36(5)	140(9)	51(5)	-1(5)	-5(4)	-13(5)
C(8)	105(9)	126(10)	50(5)	0(6)	-7(5)	-38(7)
C(9)	46(5)	120(8)	45(4)	-4(5)	3(4)	-9(5)
As(11)	35(1)	119(1)	60(1)	-3(1)	5(1)	8(1)
N(11)	63(5)	102(6)	51(4)	16(4)	21(3)	22(4)
S(11)	65(2)	133(2)	63(2)	1(2)	6(1)	23(2)
N(12)	67(5)	126(7)	59(4)	-9(5)	11(4)	24(5)
S(12)	62(2)	160(3)	50(1)	-12(2)	1(1)	15(2)
C(11)	32(4)	115(8)	33(4)	4(4)	3(3)	0(5)
C(12)	33(4)	126(9)	35(4)	2(5)	3(3)	16(5)
C(13)	45(5)	135(10)	37(4)	9(5)	-4(4)	-3(6)
C(14)	58(6)	123(9)	36(4)	-5(5)	-11(4)	1(6)
C(15)	46(5)	121(9)	34(4)	-13(5)	-3(3)	6(5)
C(16)	25(4)	133(9)	30(4)	6(5)	-4(3)	8(5)
C(17)	31(4)	115(8)	73(6)	18(6)	2(4)	4(5)
C(18)	94(9)	133(11)	57(6)	-23(6)	-8(5)	5(7)
C(19)	40(5)	112(8)	39(4)	3(4)	3(3)	9(5)

Table 2.5 Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters (Å$^2 \times 10^3$) for MesAs(S_2N_2) (**35**)

	x	y	z	U(eq)
H(3A)	-139	-1985	1029	86
H(5A)	2383	-3415	1011	80
H(7A)	-399	11	1016	113
H(7B)	442	904	850	113
H(7C)	188	522	1918	113
H(8A)	685	-4505	1504	141
H(8B)	880	-4496	377	141
H(8C)	-69	-3959	761	141
H(9A)	3719	-1065	728	105
H(9B)	3744	-2376	1148	105
H(9C)	3697	-1278	1864	105
H(13A)	4918	8809	3976	87
H(15A)	2240	9832	3872	80
H(17A)	4712	6121	3062	110
H(17B)	4766	6016	4210	110
H(17C)	5388	6970	3679	110
H(18A)	4612	10793	4216	142
H(18B)	3614	11116	4623	142
H(18C)	3793	11229	3497	142
H(19A)	1030	8631	3609	95
H(19B)	1161	7362	4091	95
H(19C)	1223	7509	2951	95

Table 2.6 Torsion angles [°] for MesAs(S_2N_2) (**35**)

C(1)−As(1)−N(1)−S(1)	−104.8(5)
S(2)−As(1)−N(1)−S(1)	1.0(4)
As(1)−N(1)−S(1)−N(2)	0.7(6)
N(1)−S(1)−N(2)−S(2)	−2.9(7)
S(1)−N(2)−S(2)−As(1)	3.1(5)
N(1)−As(1)−S(2)−N(2)	−2.2(4)
C(1)−As(1)−S(2)−N(2)	101.7(4)
N(1)−As(1)−C(1)−C(6)	−137.2(5)
S(2)−As(1)−C(1)−C(6)	128.5(5)
N(1)−As(1)−C(1)−C(2)	43.4(7)
S(2)−As(1)−C(1)−C(2)	−50.9(7)
C(6)−C(1)−C(2)−C(3)	1.1(11)
As(1)−C(1)−C(2)−C(3)	−179.5(6)
C(6)−C(1)−C(2)−C(7)	−178.5(7)
As(1)−C(1)−C(2)−C(7)	0.8(11)
C(1)−C(2)−C(3)−C(4)	0.0(12)
C(7)−C(2)−C(3)−C(4)	179.7(7)
C(2)−C(3)−C(4)−C(5)	−0.7(12)
C(2)−C(3)−C(4)−C(8)	178.2(7)
C(3)−C(4)−C(5)−C(6)	0.2(12)
C(8)−C(4)−C(5)−C(6)	−178.7(7)
C(4)−C(5)−C(6)−C(1)	0.9(11)
C(4)−C(5)−C(6)−C(9)	179.3(6)
C(2)−C(1)−C(6)−C(5)	−1.6(11)
As(1)−C(1)−C(6)−C(5)	179.0(5)
C(2)−C(1)−C(6)−C(9)	−179.8(7)
As(1)−C(1)−C(6)−C(9)	0.7(9)
C(11)−As(11)−N(11)−S(11)	−104.2(6)
S(12)−As(11)−N(11)−S(11)	2.8(5)
As(11)−N(11)−S(11)−N(12)	−2.3(8)
N(11)−S(11)−N(12)−S(12)	−0.3(9)
S(11)−N(12)−S(12)−As(11)	2.0(7)
N(11)−As(11)−S(12)−N(12)	−2.5(4)
C(11)−As(11)−S(12)−N(12)	101.1(4)
N(11)−As(11)−C(11)−C(12)	43.8(7)
S(12)−As(11)−C(11)−C(12)	−49.1(7)
N(11)−As(11)−C(11)−C(16)	−136.5(5)
S(12)−As(11)−C(11)−C(16)	130.6(5)
C(16)−C(11)−C(12)−C(13)	0.6(11)
As(11)−C(11)−C(12)−C(13)	−179.8(6)
C(16)−C(11)−C(12)−C(17)	−178.1(7)
As(11)−C(11)−C(12)−C(17)	1.6(11)
C(11)−C(12)−C(13)−C(14)	−1.2(12)
C(17)−C(12)−C(13)−C(14)	177.6(7)

Table 2.6 continued

C(12)−C(13)−C(14)−C(15)	1.4(12)
C(12)−C(13)−C(14)−C(18)	−178.3(8)
C(13)−C(14)−C(15)−C(16)	−1.0(12)
C(18)−C(14)−C(15)−C(16)	178.7(8)
C(14)−C(15)−C(16)−C(11)	0.4(12)
C(14)−C(15)−C(16)−C(19)	−179.4(7)
C(12)−C(11)−C(16)−C(15)	−0.2(11)
As(11)−C(11)−C(16)−C(15)	−179.9(6)
C(12)−C(11)−C(16)−C(19)	179.6(7)
As(11)−C(11)−C(16)−C(19)	−0.1(9)

Symmetry transformations used to generate equivalent atoms:

3 Full X-ray data of Cp*Co(S_2N_2)

Table 3.1 Crystal data and structure refinement for Cp*Co(S_2N_2) (**47**)

Identification code	vmdw13	
Empirical formula	C10 H15 Co N2 S2	
Formula weight	286.29	
Temperature	93(2) K	
Wavelength	0.710 73 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 8.1372(10) Å	$\alpha = 90°$
	b = 13.1558(16) Å	$\beta = 104.008(7)°$
	c = 12.9834(16) Å	$\gamma = 90°$
Volume	1348.6(3) Å^3	
Z	4	
Density (calculated)	1.410 Mg/m^3	
Absorption coefficient	1.554 mm^{-1}	
F(000)	592	
Crystal size	0.100 × 0.030 × 0.010 mm^3	
Theta range for data collection	2.69 to 25.35°.	
Index ranges	$-9 \leq h \leq 9, -13 \leq k \leq 15, -15 \leq l \leq 15$	
Reflections collected	11599	
Independent reflections	2372 [R(int) = 0.0675]	
Completeness to theta = 25.00°	96.6 %	
Absorption correction	Multiscan	
Max. and min. transmission	1.0000 and 0.2258	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2372 / 0 / 142	
Goodness-of-fit on F^2	1.03	
Final R indices [I>2sigma(I)]	R1 = 0.0342, wR2 = 0.0864	
R indices (all data)	R1 = 0.0357, wR2 = 0.0878	
Largest diff. peak and hole	0.401 and −0.406 e·Å^{-3}	

Table 3.2 Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for Cp*Co(S_2N_2) (**47**). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Co(1)	4067(1)	2055(1)	1890(1)	18(1)
N(1)	3925(3)	1631(2)	3247(2)	27(1)
S(1)	5353(1)	880(1)	3882(1)	28(1)
N(2)	6755(3)	589(2)	3218(2)	35(1)
S(2)	6311(1)	1176(1)	1999(1)	34(1)
C(1)	4151(3)	3119(2)	685(2)	21(1)
C(2)	3033(3)	2270(2)	252(2)	21(1)
C(3)	1669(3)	2228(2)	824(2)	22(1)
C(4)	1946(3)	3050(2)	1602(2)	23(1)
C(5)	3489(3)	3596(2)	1538(2)	22(1)
C(6)	5688(3)	3479(2)	282(2)	29(1)
C(7)	3195(3)	1568(2)	-665(2)	31(1)
C(8)	181(3)	1477(2)	591(2)	31(1)
C(9)	857(3)	3255(2)	2401(2)	31(1)
C(10)	4257(3)	4508(2)	2216(2)	28(1)

Table 3.3 Bond lengths [Å] and angles [°] for Cp*Co(S_2N_2) (**47**)

Co(1)−N(1)	1.8780(19)
Co(1)−C(5)	2.106(2)
Co(1)−C(2)	2.108(2)
Co(1)−C(1)	2.113(2)
Co(1)−C(3)	2.113(2)
Co(1)−C(4)	2.126(2)
Co(1)−S(2)	2.1371(7)
N(1)−S(1)	1.594(2)
S(1)−N(2)	1.634(2)
N(2)−S(2)	1.718(2)
C(1)−C(2)	1.465(3)
C(1)−C(5)	1.482(3)
C(1)−C(6)	1.542(3)
C(2)−C(3)	1.479(3)
C(2)−C(7)	1.537(3)
C(3)−C(4)	1.460(3)
C(3)−C(8)	1.535(3)
C(4)−C(5)	1.466(3)
C(4)−C(9)	1.542(3)
C(5)−C(10)	1.530(3)
C(6)−H(6A)	0.9800
C(6)−H(6B)	0.9800
C(6)−H(6C)	0.9800
C(7)−H(7A)	0.9800
C(7)−H(7B)	0.9800
C(7)−H(7C)	0.9800
C(8)−H(8A)	0.9800
C(8)−H(8B)	0.9800
C(8)−H(8C)	0.9800
C(9)−H(9A)	0.9800
C(9)−H(9B)	0.9800
C(9)−H(9C)	0.9800
C(10)−H(10A)	0.9800
C(10)−H(10B)	0.9800
C(10)−H(10C)	0.9800
N(1)−Co(1)−C(5)	115.38(9)
N(1)−Co(1)−C(2)	152.39(9)
C(5)−Co(1)−C(2)	68.80(9)
N(1)−Co(1)−C(1)	155.76(9)
C(5)−Co(1)−C(1)	41.14(8)
C(2)−Co(1)−C(1)	40.60(9)
N(1)−Co(1)−C(3)	112.94(9)
C(5)−Co(1)−C(3)	68.42(9)

Table 3.3 continued

C(2)−Co(1)−C(3)	41.00(8)
C(1)−Co(1)−C(3)	68.54(9)
N(1)−Co(1)−C(4)	96.68(9)
C(5)−Co(1)−C(4)	40.55(9)
C(2)−Co(1)−C(4)	68.38(9)
C(1)−Co(1)−C(4)	68.43(8)
C(3)−Co(1)−C(4)	40.29(9)
N(1)−Co(1)−S(2)	91.29(6)
C(5)−Co(1)−S(2)	132.63(6)
C(2)−Co(1)−S(2)	105.39(6)
C(1)−Co(1)−S(2)	103.13(6)
C(3)−Co(1)−S(2)	137.76(7)
C(4)−Co(1)−S(2)	171.56(6)
S(1)−N(1)−Co(1)	117.83(11)
N(1)−S(1)−N(2)	112.75(11)
S(1)−N(2)−S(2)	111.27(12)
N(2)−S(2)−Co(1)	106.86(8)
C(2)−C(1)−C(5)	107.78(18)
C(2)−C(1)−C(6)	125.7(2)
C(5)−C(1)−C(6)	126.5(2)
C(2)−C(1)−Co(1)	69.53(12)
C(5)−C(1)−Co(1)	69.16(12)
C(6)−C(1)−Co(1)	128.95(16)
C(1)−C(2)−C(3)	107.90(19)
C(1)−C(2)−C(7)	126.41(19)
C(3)−C(2)−C(7)	125.6(2)
C(1)−C(2)−Co(1)	69.86(12)
C(3)−C(2)−Co(1)	69.67(12)
C(7)−C(2)−Co(1)	127.80(17)
C(4)−C(3)−C(2)	108.14(19)
C(4)−C(3)−C(8)	126.6(2)
C(2)−C(3)−C(8)	125.2(2)
C(4)−C(3)−Co(1)	70.32(12)
C(2)−C(3)−Co(1)	69.33(12)
C(8)−C(3)−Co(1)	128.26(16)
C(3)−C(4)−C(5)	108.30(19)
C(3)−C(4)−C(9)	125.3(2)
C(5)−C(4)−C(9)	126.3(2)
C(3)−C(4)−Co(1)	69.39(12)
C(5)−C(4)−Co(1)	68.98(12)
C(9)−C(4)−Co(1)	124.30(16)
C(4)−C(5)−C(1)	107.85(19)
C(4)−C(5)−C(10)	126.0(2)
C(1)−C(5)−C(10)	126.2(2)

Table 3.3 continued

C(4)−C(5)−Co(1)	70.47(12)
C(1)−C(5)−Co(1)	69.70(12)
C(10)−C(5)−Co(1)	126.29(16)
C(1)−C(6)−H(6A)	109.5
C(1)−C(6)−H(6B)	109.5
H(6A)−C(6)−H(6B)	109.5
C(1)−C(6)−H(6C)	109.5
H(6A)−C(6)−H(6C)	109.5
H(6B)−C(6)−H(6C)	109.5
C(2)−C(7)−H(7A)	109.5
C(2)−C(7)−H(7B)	109.5
H(7A)−C(7)−H(7B)	109.5
C(2)−C(7)−H(7C)	109.5
H(7A)−C(7)−H(7C)	109.5
H(7B)−C(7)−H(7C)	109.5
C(3)−C(8)−H(8A)	109.5
C(3)−C(8)−H(8B)	109.5
H(8A)−C(8)−H(8B)	109.5
C(3)−C(8)−H(8C)	109.5
H(8A)−C(8)−H(8C)	109.5
H(8B)−C(8)−H(8C)	109.5
C(4)−C(9)−H(9A)	109.5
C(4)−C(9)−H(9B)	109.5
H(9A)−C(9)−H(9B)	109.5
C(4)−C(9)−H(9C)	109.5
H(9A)−C(9)−H(9C)	109.5
H(9B)−C(9)−H(9C)	109.5
C(5)−C(10)−H(10A)	109.5
C(5)−C(10)−H(10B)	109.5
H(10A)−C(10)−H(10B)	109.5
C(5)−C(10)−H(10C)	109.5
H(10A)−C(10)−H(10C)	109.5
H(10B)−C(10)−H(10C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 3.4 Anisotropic displacement parameters (Å$^2\times10^3$) for Cp*Co(S_2N_2) (**47**). The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2\ a^{*2}\ U^{11} + \ldots + 2\ h\ k\ a^*\ b^*\ U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Co(1)	18(1)	20(1)	18(1)	2(1)	5(1)	2(1)
N(1)	30(1)	29(1)	22(1)	3(1)	8(1)	2(1)
S(1)	33(1)	27(1)	22(1)	5(1)	0(1)	0(1)
N(2)	30(1)	31(1)	40(1)	9(1)	2(1)	7(1)
S(2)	29(1)	39(1)	39(1)	11(1)	16(1)	14(1)
C(1)	21(1)	23(1)	19(1)	5(1)	5(1)	2(1)
C(2)	21(1)	24(1)	18(1)	2(1)	4(1)	0(1)
C(3)	20(1)	25(1)	20(1)	5(1)	3(1)	3(1)
C(4)	22(1)	26(1)	22(1)	6(1)	6(1)	5(1)
C(5)	24(1)	21(1)	20(1)	3(1)	4(1)	4(1)
C(6)	27(1)	30(1)	31(1)	4(1)	11(1)	-3(1)
C(7)	37(1)	33(1)	23(1)	-7(1)	11(1)	-4(1)
C(8)	24(1)	35(1)	32(1)	4(1)	5(1)	-6(1)
C(9)	29(1)	35(1)	33(1)	4(1)	15(1)	10(1)
C(10)	32(1)	23(1)	30(1)	-1(1)	6(1)	1(1)

Table 3.5 Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters (Å$^2 \times 10^3$) for Cp*Co(S_2N_2) (**47**)

	x	y	z	U(eq)
H(6A)	6235	2891	43	43
H(6B)	6498	3823	859	43
H(6C)	5307	3951	-311	43
H(7A)	2570	1862	-1341	46
H(7B)	2728	898	-570	46
H(7C)	4393	1498	-670	46
H(8A)	-304	1430	1211	46
H(8B)	584	805	436	46
H(8C)	-687	1715	-23	46
H(9A)	-247	3524	2024	46
H(9B)	1432	3751	2930	46
H(9C)	696	2619	2758	46
H(10A)	3639	5126	1932	43
H(10B)	5450	4580	2202	43
H(10C)	4175	4403	2949	43

Table 3.6 Torsion angles [°] for Cp*Co(S_2N_2) (**47**)

C(5)−Co(1)−N(1)−S(1)	−139.23(12)
C(2)−Co(1)−N(1)−S(1)	128.27(17)
C(1)−Co(1)−N(1)−S(1)	−126.86(19)
C(3)−Co(1)−N(1)−S(1)	144.72(12)
C(4)−Co(1)−N(1)−S(1)	−176.94(13)
S(2)−Co(1)−N(1)−S(1)	0.27(12)
Co(1)−N(1)−S(1)−N(2)	−0.20(17)
N(1)−S(1)−N(2)−S(2)	−0.02(18)
S(1)−N(2)−S(2)−Co(1)	0.20(15)
N(1)−Co(1)−S(2)−N(2)	−0.26(11)
C(5)−Co(1)−S(2)−N(2)	126.86(12)
C(2)−Co(1)−S(2)−N(2)	−158.00(11)
C(1)−Co(1)−S(2)−N(2)	160.10(11)
C(3)−Co(1)−S(2)−N(2)	−127.47(12)
C(4)−Co(1)−S(2)−N(2)	160.5(5)
N(1)−Co(1)−C(1)−C(2)	−136.5(2)
C(5)−Co(1)−C(1)−C(2)	−119.40(18)
C(3)−Co(1)−C(1)−C(2)	−38.06(13)
C(4)−Co(1)−C(1)−C(2)	−81.52(14)
S(2)−Co(1)−C(1)−C(2)	98.42(12)
N(1)−Co(1)−C(1)−C(5)	−17.1(3)
C(2)−Co(1)−C(1)−C(5)	119.40(18)
C(3)−Co(1)−C(1)−C(5)	81.34(14)
C(4)−Co(1)−C(1)−C(5)	37.88(13)
S(2)−Co(1)−C(1)−C(5)	−142.18(12)
N(1)−Co(1)−C(1)−C(6)	103.6(3)
C(5)−Co(1)−C(1)−C(6)	120.7(3)
C(2)−Co(1)−C(1)−C(6)	−119.9(3)
C(3)−Co(1)−C(1)−C(6)	−158.0(2)
C(4)−Co(1)−C(1)−C(6)	158.6(2)
S(2)−Co(1)−C(1)−C(6)	−21.5(2)
C(5)−C(1)−C(2)−C(3)	0.7(2)
C(6)−C(1)−C(2)−C(3)	−176.6(2)
Co(1)−C(1)−C(2)−C(3)	59.51(15)
C(5)−C(1)−C(2)−C(7)	178.5(2)
C(6)−C(1)−C(2)−C(7)	1.2(4)
Co(1)−C(1)−C(2)−C(7)	−122.7(2)
C(5)−C(1)−C(2)−Co(1)	−58.77(15)
C(6)−C(1)−C(2)−Co(1)	123.9(2)
N(1)−Co(1)−C(2)−C(1)	142.44(18)
C(5)−Co(1)−C(2)−C(1)	37.94(13)
C(3)−Co(1)−C(2)−C(1)	119.02(18)
C(4)−Co(1)−C(2)−C(1)	81.64(14)
S(2)−Co(1)−C(2)−C(1)	−92.35(12)

Table 3.6 continued

N(1)−Co(1)−C(2)−C(3)	23.4(2)
C(5)−Co(1)−C(2)−C(3)	−81.08(14)
C(1)−Co(1)−C(2)−C(3)	−119.02(18)
C(4)−Co(1)−C(2)−C(3)	−37.37(13)
S(2)−Co(1)−C(2)−C(3)	148.63(11)
N(1)−Co(1)−C(2)−C(7)	−96.5(3)
C(5)−Co(1)−C(2)−C(7)	159.0(2)
C(1)−Co(1)−C(2)−C(7)	121.0(2)
C(3)−Co(1)−C(2)−C(7)	−119.9(3)
C(4)−Co(1)−C(2)−C(7)	−157.3(2)
S(2)−Co(1)−C(2)−C(7)	28.7(2)
C(1)−C(2)−C(3)−C(4)	0.2(2)
C(7)−C(2)−C(3)−C(4)	−177.6(2)
Co(1)−C(2)−C(3)−C(4)	59.85(15)
C(1)−C(2)−C(3)−C(8)	177.4(2)
C(7)−C(2)−C(3)−C(8)	−0.4(4)
Co(1)−C(2)−C(3)−C(8)	−122.9(2)
C(1)−C(2)−C(3)−Co(1)	−59.63(15)
C(7)−C(2)−C(3)−Co(1)	122.6(2)
N(1)−Co(1)−C(3)−C(4)	72.31(14)
C(5)−Co(1)−C(3)−C(4)	−37.15(12)
C(2)−Co(1)−C(3)−C(4)	−119.23(18)
C(1)−Co(1)−C(3)−C(4)	−81.53(13)
S(2)−Co(1)−C(3)−C(4)	−167.53(10)
N(1)−Co(1)−C(3)−C(2)	−168.46(13)
C(5)−Co(1)−C(3)−C(2)	82.08(14)
C(1)−Co(1)−C(3)−C(2)	37.70(13)
C(4)−Co(1)−C(3)−C(2)	119.23(18)
S(2)−Co(1)−C(3)−C(2)	−48.30(16)
N(1)−Co(1)−C(3)−C(8)	−49.3(2)
C(5)−Co(1)−C(3)−C(8)	−158.7(2)
C(2)−Co(1)−C(3)−C(8)	119.2(3)
C(1)−Co(1)−C(3)−C(8)	156.9(2)
C(4)−Co(1)−C(3)−C(8)	−121.6(3)
S(2)−Co(1)−C(3)−C(8)	70.9(2)
C(2)−C(3)−C(4)−C(5)	−1.1(2)
C(8)−C(3)−C(4)−C(5)	−178.3(2)
Co(1)−C(3)−C(4)−C(5)	58.13(15)
C(2)−C(3)−C(4)−C(9)	−177.4(2)
C(8)−C(3)−C(4)−C(9)	5.5(4)
Co(1)−C(3)−C(4)−C(9)	−118.1(2)
C(2)−C(3)−C(4)−Co(1)	−59.23(15)
C(8)−C(3)−C(4)−Co(1)	123.6(2)
N(1)−Co(1)−C(4)−C(3)	−117.95(13)

Table 3.6 continued

C(5)−Co(1)−C(4)−C(3)	120.26(18)
C(2)−Co(1)−C(4)−C(3)	38.02(12)
C(1)−Co(1)−C(4)−C(3)	81.84(13)
S(2)−Co(1)−C(4)−C(3)	81.4(5)
N(1)−Co(1)−C(4)−C(5)	121.79(13)
C(2)−Co(1)−C(4)−C(5)	−82.24(13)
C(1)−Co(1)−C(4)−C(5)	−38.42(13)
C(3)−Co(1)−C(4)−C(5)	−120.26(18)
S(2)−Co(1)−C(4)−C(5)	−38.8(5)
N(1)−Co(1)−C(4)−C(9)	1.4(2)
C(5)−Co(1)−C(4)−C(9)	−120.4(3)
C(2)−Co(1)−C(4)−C(9)	157.4(2)
C(1)−Co(1)−C(4)−C(9)	−158.8(2)
C(3)−Co(1)−C(4)−C(9)	119.4(3)
S(2)−Co(1)−C(4)−C(9)	−159.2(4)
C(3)−C(4)−C(5)−C(1)	1.5(2)
C(9)−C(4)−C(5)−C(1)	177.8(2)
Co(1)−C(4)−C(5)−C(1)	59.93(15)
C(3)−C(4)−C(5)−C(10)	−179.6(2)
C(9)−C(4)−C(5)−C(10)	−3.4(4)
Co(1)−C(4)−C(5)−C(10)	−121.2(2)
C(3)−C(4)−C(5)−Co(1)	−58.38(15)
C(9)−C(4)−C(5)−Co(1)	117.8(2)
C(2)−C(1)−C(5)−C(4)	−1.4(2)
C(6)−C(1)−C(5)−C(4)	175.9(2)
Co(1)−C(1)−C(5)−C(4)	−60.41(15)
C(2)−C(1)−C(5)−C(10)	179.8(2)
C(6)−C(1)−C(5)−C(10)	−3.0(4)
Co(1)−C(1)−C(5)−C(10)	120.8(2)
C(2)−C(1)−C(5)−Co(1)	59.00(15)
C(6)−C(1)−C(5)−Co(1)	−123.7(2)
N(1)−Co(1)−C(5)−C(4)	−69.12(15)
C(2)−Co(1)−C(5)−C(4)	81.11(14)
C(1)−Co(1)−C(5)−C(4)	118.56(18)
C(3)−Co(1)−C(5)−C(4)	36.92(13)
S(2)−Co(1)−C(5)−C(4)	172.81(10)
N(1)−Co(1)−C(5)−C(1)	172.31(12)
C(2)−Co(1)−C(5)−C(1)	−37.46(13)
C(3)−Co(1)−C(5)−C(1)	−81.65(14)
C(4)−Co(1)−C(5)−C(1)	−118.56(18)
S(2)−Co(1)−C(5)−C(1)	54.25(15)
N(1)−Co(1)−C(5)−C(10)	51.7(2)
C(2)−Co(1)−C(5)−C(10)	−158.0(2)
C(1)−Co(1)−C(5)−C(10)	−120.6(2)

Table 3.6 continued

C(3)−Co(1)−C(5)−C(10)	157.8(2)
C(4)−Co(1)−C(5)−C(10)	120.9(2)
S(2)−Co(1)−C(5)−C(10)	−66.3(2)

Symmetry transformations used to generate equivalent atoms:

4 Full X-ray data of Cp*Ir(S_2N_2)

Table 4.1 Crystal data and structure refinement for Cp*Ir(S_2N_2) (**51**)

Identification code	vmdw6	
Empirical formula	C10 H15 Ir N2 S2	
Formula weight	419.56	
Temperature	93(2) K	
Wavelength	0.710 73 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 7.856(3) Å	$\alpha = 90°$
	b = 13.129(5) Å	$\beta = 103.39(3)°$
	c = 12.860(13) Å	$\gamma = 90°$
Volume	1290.4(14) $Å^3$	
Z	4	
Density (calculated)	2.160 Mg/m^3	
Absorption coefficient	10.641 mm^{-1}	
F(000)	792	
Crystal size	0.1000 × 0.1000 × 0.0100 mm^3	
Theta range for data collection	3.08 to 25.43°	
Index ranges	$-9 \leq h \leq 5, -15 \leq k \leq 15, -15 \leq l \leq 13$	
Reflections collected	7725	
Independent reflections	2296 [R(int) = 0.0426]	
Completeness to theta = 25.00°	96.9 %	
Absorption correction	Multiscan	
Max. and min. transmission	1.0000 and 0.1902	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2296 / 0 / 142	
Goodness-of-fit on F^2	0.853	
Final R indices [I>2sigma(I)]	R1 = 0.0217, wR2 = 0.0416	
R indices (all data)	R1 = 0.0236, wR2 = 0.0421	
Largest diff. peak and hole	1.051 and −0.825 e·$Å^{-3}$	

Table 4.2 Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters (Å$^2 \times 10^3$) for Cp*Ir(S_2N_2) (**51**). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ir(1)	4100(1)	1974(1)	1897(1)	10(1)
N(1)	4031(5)	1553(3)	3351(2)	20(1)
S(1)	5464(1)	803(1)	3959(1)	21(1)
N(2)	6826(5)	470(3)	3289(2)	24(1)
S(2)	6417(1)	1006(1)	2068(1)	23(1)
C(1)	4057(6)	3099(3)	623(3)	14(1)
C(2)	2929(5)	2272(3)	203(3)	15(1)
C(3)	1579(5)	2207(3)	790(3)	15(1)
C(4)	1843(6)	3012(3)	1566(3)	15(1)
C(5)	3365(5)	3560(3)	1485(3)	13(1)
C(6)	5566(5)	3486(3)	214(3)	19(1)
C(7)	3080(6)	1599(3)	-719(3)	22(1)
C(8)	75(5)	1479(3)	548(3)	22(1)
C(9)	723(6)	3215(3)	2347(3)	23(1)
C(10)	4124(5)	4438(3)	2118(3)	20(1)

Table 4.3 Bond lengths [Å] and angles [°] for Cp*Ir(S_2N_2) (**51**)

Ir(1)−N(1)	1.963(3)
Ir(1)−C(3)	2.177(4)
Ir(1)−S(2)	2.1891(12)
Ir(1)−C(5)	2.192(4)
Ir(1)−C(2)	2.194(4)
Ir(1)−C(4)	2.198(4)
Ir(1)−C(1)	2.201(4)
N(1)−S(1)	1.562(4)
S(1)−N(2)	1.583(4)
N(2)−S(2)	1.682(3)
C(1)−C(2)	1.426(6)
C(1)−C(5)	1.474(5)
C(1)−C(6)	1.493(5)
C(2)−C(3)	1.440(5)
C(2)−C(7)	1.505(5)
C(3)−C(4)	1.435(5)
C(3)−C(8)	1.495(6)
C(4)−C(5)	1.419(6)
C(4)−C(9)	1.506(5)
C(5)−C(10)	1.457(6)
N(1)−Ir(1)−C(3)	116.18(15)
N(1)−Ir(1)−S(2)	86.94(11)
C(3)−Ir(1)−S(2)	139.19(11)
N(1)−Ir(1)−C(5)	115.72(14)
C(3)−Ir(1)−C(5)	63.87(15)
S(2)−Ir(1)−C(5)	137.89(11)
N(1)−Ir(1)−C(2)	153.92(15)
C(3)−Ir(1)−C(2)	38.46(14)
S(2)−Ir(1)−C(2)	110.51(11)
C(5)−Ir(1)−C(2)	64.20(14)
N(1)−Ir(1)−C(4)	99.24(14)
C(3)−Ir(1)−C(4)	38.29(14)
S(2)−Ir(1)−C(4)	173.71(10)
C(5)−Ir(1)−C(4)	37.72(14)
C(2)−Ir(1)−C(4)	64.11(14)
N(1)−Ir(1)−C(1)	154.12(15)
C(3)−Ir(1)−C(1)	64.14(15)
S(2)−Ir(1)−C(1)	109.45(11)
C(5)−Ir(1)−C(1)	39.21(13)
C(2)−Ir(1)−C(1)	37.87(15)
C(4)−Ir(1)−C(1)	64.35(15)
S(1)−N(1)−Ir(1)	118.59(19)
N(1)−S(1)−N(2)	113.67(17)

Table 4.3 continued

S(1)−N(2)−S(2)	112.7(2)
N(2)−S(2)−Ir(1)	108.13(13)
C(2)−C(1)−C(5)	107.0(3)
C(2)−C(1)−C(6)	126.9(3)
C(5)−C(1)−C(6)	125.9(4)
C(2)−C(1)−Ir(1)	70.8(2)
C(5)−C(1)−Ir(1)	70.1(2)
C(6)−C(1)−Ir(1)	127.9(3)
C(1)−C(2)−C(3)	108.4(3)
C(1)−C(2)−C(7)	126.1(4)
C(3)−C(2)−C(7)	125.5(4)
C(1)−C(2)−Ir(1)	71.3(2)
C(3)−C(2)−Ir(1)	70.1(2)
C(7)−C(2)−Ir(1)	125.9(3)
C(4)−C(3)−C(2)	108.4(4)
C(4)−C(3)−C(8)	126.6(4)
C(2)−C(3)−C(8)	124.8(4)
C(4)−C(3)−Ir(1)	71.7(2)
C(2)−C(3)−Ir(1)	71.4(2)
C(8)−C(3)−Ir(1)	127.0(3)
C(5)−C(4)−C(3)	108.1(3)
C(5)−C(4)−C(9)	126.3(3)
C(3)−C(4)−C(9)	125.6(4)
C(5)−C(4)−Ir(1)	70.9(2)
C(3)−C(4)−Ir(1)	70.0(2)
C(9)−C(4)−Ir(1)	123.4(3)
C(4)−C(5)−C(10)	127.1(3)
C(4)−C(5)−C(1)	108.1(3)
C(10)−C(5)−C(1)	124.8(4)
C(4)−C(5)−Ir(1)	71.4(2)
C(10)−C(5)−Ir(1)	124.5(3)
C(1)−C(5)−Ir(1)	70.7(2)

Symmetry transformations used to generate equivalent atoms:

Table 4.4 Anisotropic displacement parameters ($Å^2 \times 10^3$) for Cp*Ir(S_2N_2) (**51**). The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2\ a^{*2}\ U^{11} + \ldots + 2\ h\ k\ a^*\ b^*\ U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ir(1)	11(1)	12(1)	10(1)	1(1)	3(1)	1(1)
N(1)	22(2)	25(2)	12(2)	2(2)	5(1)	0(2)
S(1)	23(1)	23(1)	14(1)	5(1)	-1(1)	-2(1)
N(2)	21(2)	23(2)	25(2)	7(2)	0(2)	5(2)
S(2)	21(1)	25(1)	25(1)	7(1)	10(1)	11(1)
C(1)	14(2)	16(3)	10(2)	6(2)	2(2)	3(2)
C(2)	14(2)	21(2)	8(2)	2(2)	2(2)	2(2)
C(3)	9(2)	20(2)	16(2)	6(2)	0(2)	1(2)
C(4)	15(3)	19(3)	11(2)	0(2)	5(2)	4(2)
C(5)	19(2)	8(2)	13(2)	5(2)	4(2)	6(2)
C(6)	17(2)	20(3)	21(2)	5(2)	7(2)	-2(2)
C(7)	28(3)	16(3)	20(2)	-5(2)	6(2)	1(2)
C(8)	16(3)	26(3)	25(2)	2(2)	5(2)	-5(2)
C(9)	19(3)	28(3)	25(2)	4(2)	13(2)	8(2)
C(10)	10(2)	29(3)	21(2)	16(2)	4(2)	0(2)

Table 4.5 Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($Å^2 \times 10^3$) for Cp*Ir(S_2N_2) (**51**)

	x	y	z	U(eq)
H(6A)	6120	2917	-76	28
H(6B)	6421	3805	800	28
H(6C)	5149	3989	-350	28
H(7A)	2434	1905	-1390	33
H(7B)	2589	927	-632	33
H(7C)	4314	1526	-737	33
H(8A)	-422	1411	1176	34
H(8B)	485	812	364	34
H(8C)	-822	1736	-56	34
H(9A)	1371	3642	2932	34
H(9B)	417	2568	2637	34
H(9C)	-348	3568	1982	34
H(10A)	3541	5060	1796	30
H(10B)	5376	4478	2134	30
H(10C)	3967	4367	2848	30

Table 4.6 Torsion angles [°] for Cp*Ir(S_2N_2) (**51**)

C(3)−Ir(1)−N(1)−S(1)	145.1(2)
S(2)−Ir(1)−N(1)−S(1)	0.1(2)
C(5)−Ir(1)−N(1)−S(1)	−142.9(2)
C(2)−Ir(1)−N(1)−S(1)	133.7(3)
C(4)−Ir(1)−N(1)−S(1)	−178.7(2)
C(1)−Ir(1)−N(1)−S(1)	−130.7(3)
Ir(1)−N(1)−S(1)−N(2)	−0.2(3)
N(1)−S(1)−N(2)−S(2)	0.1(3)
S(1)−N(2)−S(2)−Ir(1)	0.0(2)
N(1)−Ir(1)−S(2)−N(2)	−0.08(17)
C(3)−Ir(1)−S(2)−N(2)	−128.0(2)
C(5)−Ir(1)−S(2)−N(2)	126.00(19)
C(2)−Ir(1)−S(2)−N(2)	−160.20(18)
C(4)−Ir(1)−S(2)−N(2)	169.1(10)
C(1)−Ir(1)−S(2)−N(2)	159.42(18)
N(1)−Ir(1)−C(1)−C(2)	−134.5(3)
C(3)−Ir(1)−C(1)−C(2)	−37.4(2)
S(2)−Ir(1)−C(1)−C(2)	98.7(2)
C(5)−Ir(1)−C(1)−C(2)	−117.1(3)
C(4)−Ir(1)−C(1)−C(2)	−80.1(3)
N(1)−Ir(1)−C(1)−C(5)	−17.5(5)
C(3)−Ir(1)−C(1)−C(5)	79.6(2)
S(2)−Ir(1)−C(1)−C(5)	−144.3(2)
C(2)−Ir(1)−C(1)−C(5)	117.1(3)
C(4)−Ir(1)−C(1)−C(5)	36.9(2)
N(1)−Ir(1)−C(1)−C(6)	103.1(4)
C(3)−Ir(1)−C(1)−C(6)	−159.8(4)
S(2)−Ir(1)−C(1)−C(6)	−23.7(4)
C(5)−Ir(1)−C(1)−C(6)	120.6(4)
C(2)−Ir(1)−C(1)−C(6)	−122.4(5)
C(4)−Ir(1)−C(1)−C(6)	157.5(4)
C(5)−C(1)−C(2)−C(3)	−0.5(4)
C(6)−C(1)−C(2)−C(3)	−175.9(4)
Ir(1)−C(1)−C(2)−C(3)	60.6(3)
C(5)−C(1)−C(2)−C(7)	177.6(4)
C(6)−C(1)−C(2)−C(7)	2.2(6)
Ir(1)−C(1)−C(2)−C(7)	−121.3(4)
C(5)−C(1)−C(2)−Ir(1)	−61.1(2)
C(6)−C(1)−C(2)−Ir(1)	123.5(4)
N(1)−Ir(1)−C(2)−C(1)	134.9(3)
C(3)−Ir(1)−C(2)−C(1)	118.5(4)
S(2)−Ir(1)−C(2)−C(1)	−95.6(2)
C(5)−Ir(1)−C(2)−C(1)	38.7(2)
C(4)−Ir(1)−C(2)−C(1)	80.8(3)

Table 4.6 continued

N(1)−Ir(1)−C(2)−C(3)	16.5(5)
S(2)−Ir(1)−C(2)−C(3)	145.9(2)
C(5)−Ir(1)−C(2)−C(3)	−79.8(3)
C(4)−Ir(1)−C(2)−C(3)	−37.7(2)
C(1)−Ir(1)−C(2)−C(3)	−118.5(4)
N(1)−Ir(1)−C(2)−C(7)	−103.5(4)
C(3)−Ir(1)−C(2)−C(7)	−120.0(5)
S(2)−Ir(1)−C(2)−C(7)	25.9(4)
C(5)−Ir(1)−C(2)−C(7)	160.3(4)
C(4)−Ir(1)−C(2)−C(7)	−157.6(4)
C(1)−Ir(1)−C(2)−C(7)	121.6(5)
C(1)−C(2)−C(3)−C(4)	1.2(4)
C(7)−C(2)−C(3)−C(4)	−176.9(4)
Ir(1)−C(2)−C(3)−C(4)	62.5(3)
C(1)−C(2)−C(3)−C(8)	176.0(4)
C(7)−C(2)−C(3)−C(8)	−2.1(6)
Ir(1)−C(2)−C(3)−C(8)	−122.6(4)
C(1)−C(2)−C(3)−Ir(1)	−61.3(3)
C(7)−C(2)−C(3)−Ir(1)	120.5(4)
N(1)−Ir(1)−C(3)−C(4)	70.5(3)
S(2)−Ir(1)−C(3)−C(4)	−170.94(17)
C(5)−Ir(1)−C(3)−C(4)	−36.8(2)
C(2)−Ir(1)−C(3)−C(4)	−117.5(3)
C(1)−Ir(1)−C(3)−C(4)	−80.7(3)
N(1)−Ir(1)−C(3)−C(2)	−172.0(2)
S(2)−Ir(1)−C(3)−C(2)	−53.4(3)
C(5)−Ir(1)−C(3)−C(2)	80.7(2)
C(4)−Ir(1)−C(3)−C(2)	117.5(3)
C(1)−Ir(1)−C(3)−C(2)	36.9(2)
N(1)−Ir(1)−C(3)−C(8)	−51.9(4)
S(2)−Ir(1)−C(3)−C(8)	66.6(4)
C(5)−Ir(1)−C(3)−C(8)	−159.2(4)
C(2)−Ir(1)−C(3)−C(8)	120.1(5)
C(4)−Ir(1)−C(3)−C(8)	−122.4(4)
C(1)−Ir(1)−C(3)−C(8)	156.9(4)
C(2)−C(3)−C(4)−C(5)	−1.4(4)
C(8)−C(3)−C(4)−C(5)	−176.1(4)
Ir(1)−C(3)−C(4)−C(5)	61.0(3)
C(2)−C(3)−C(4)−C(9)	−179.8(4)
C(8)−C(3)−C(4)−C(9)	5.5(6)
Ir(1)−C(3)−C(4)−C(9)	−117.4(4)
C(2)−C(3)−C(4)−Ir(1)	−62.4(3)
C(8)−C(3)−C(4)−Ir(1)	122.9(4)
N(1)−Ir(1)−C(4)−C(5)	120.5(2)

Table 4.6 continued

C(3)−Ir(1)−C(4)−C(5)	−118.4(3)
S(2)−Ir(1)−C(4)−C(5)	−48.5(11)
C(2)−Ir(1)−C(4)−C(5)	−80.6(2)
C(1)−Ir(1)−C(4)−C(5)	−38.4(2)
N(1)−Ir(1)−C(4)−C(3)	−121.0(2)
S(2)−Ir(1)−C(4)−C(3)	69.9(11)
C(5)−Ir(1)−C(4)−C(3)	118.4(3)
C(2)−Ir(1)−C(4)−C(3)	37.8(2)
C(1)−Ir(1)−C(4)−C(3)	80.1(2)
N(1)−Ir(1)−C(4)−C(9)	−0.9(4)
C(3)−Ir(1)−C(4)−C(9)	120.1(4)
S(2)−Ir(1)−C(4)−C(9)	−170.0(8)
C(5)−Ir(1)−C(4)−C(9)	−121.4(4)
C(2)−Ir(1)−C(4)−C(9)	157.9(4)
C(1)−Ir(1)−C(4)−C(9)	−159.8(4)
C(3)−C(4)−C(5)−C(10)	179.9(4)
C(9)−C(4)−C(5)−C(10)	−1.7(7)
Ir(1)−C(4)−C(5)−C(10)	−119.6(4)
C(3)−C(4)−C(5)−C(1)	1.1(4)
C(9)−C(4)−C(5)−C(1)	179.4(4)
Ir(1)−C(4)−C(5)−C(1)	61.5(3)
C(3)−C(4)−C(5)−Ir(1)	−60.4(3)
C(9)−C(4)−C(5)−Ir(1)	117.9(4)
C(2)−C(1)−C(5)−C(4)	−0.3(4)
C(6)−C(1)−C(5)−C(4)	175.1(4)
Ir(1)−C(1)−C(5)−C(4)	−61.9(3)
C(2)−C(1)−C(5)−C(10)	−179.2(4)
C(6)−C(1)−C(5)−C(10)	−3.8(6)
Ir(1)−C(1)−C(5)−C(10)	119.2(4)
C(2)−C(1)−C(5)−Ir(1)	61.6(3)
C(6)−C(1)−C(5)−Ir(1)	−123.0(4)
N(1)−Ir(1)−C(5)−C(4)	−70.6(2)
C(3)−Ir(1)−C(5)−C(4)	37.4(2)
S(2)−Ir(1)−C(5)−C(4)	172.97(16)
C(2)−Ir(1)−C(5)−C(4)	80.3(2)
C(1)−Ir(1)−C(5)−C(4)	117.7(3)
N(1)−Ir(1)−C(5)−C(10)	52.1(4)
C(3)−Ir(1)−C(5)−C(10)	160.1(4)
S(2)−Ir(1)−C(5)−C(10)	−64.3(4)
C(2)−Ir(1)−C(5)−C(10)	−156.9(4)
C(4)−Ir(1)−C(5)−C(10)	122.7(4)
C(1)−Ir(1)−C(5)−C(10)	−119.5(4)
N(1)−Ir(1)−C(5)−C(1)	171.6(2)
C(3)−Ir(1)−C(5)−C(1)	−80.4(2)

Table 4.6 continued

S(2)−Ir(1)−C(5)−C(1)	55.2(3)
C(2)−Ir(1)−C(5)−C(1)	−37.4(2)
C(4)−Ir(1)−C(5)−C(1)	−117.7(3)

Symmetry transformations used to generate equivalent atoms:

5 Full X-ray data of [Cp*RhCp*]Cl · H_2O

Table 5.1 Crystal data and structure refinement for [Cp*RhCp*]Cl · H_2O (**52**)

Identification code	vmdw39	
Empirical formula	C20 H32 Cl O Rh	
Formula weight	426.82	
Temperature	93(2) K	
Wavelength	0.710 73 Å	
Crystal system	Monoclinic	
Space group	C2/m	
Unit cell dimensions	a = 16.909(3) Å	$\alpha = 90°$
	b = 10.1450(17) Å	$\beta = 124.929(9)°$
	c = 13.854(3) Å	$\gamma = 90°$
Volume	1948.4(6) $Å^3$	
Z	4	
Density (calculated)	1.455 Mg/m^3	
Absorption coefficient	1.016 mm^{-1}	
F(000)	888	
Crystal size	0.150 × 0.100 × 0.030 mm^3	
Theta range for data collection	2.41 to 25.35°	
Index ranges	$-18 \leq h \leq 20, -12 \leq k \leq 11, -15 \leq l \leq 15$	
Reflections collected	5759	
Independent reflections	1646 [R(int) = 0.0703]	
Completeness to theta = 25.00°	87.2 %	
Absorption correction	Multiscan	
Max. and min. transmission	1.0000 and 0.9821	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1646 / 2 / 127	
Goodness-of-fit on F^2	1.07	
Final R indices [I>2sigma(I)]	R1 = 0.0347, wR2 = 0.0870	
R indices (all data)	R1 = 0.0363, wR2 = 0.0878	
Extinction coefficient	0.007(3)	
Largest diff. peak and hole	0.606 and −0.582 e·$Å^{-3}$	

Table 5.2 Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for [Cp*RhCp*]Cl · H_2O (**52**). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Rh(1)	2478(1)	0	2654(1)	11(1)
C(1)	3922(2)	-707(3)	3285(2)	13(1)
C(2)	3679(2)	-1158(3)	4078(2)	15(1)
C(3)	3526(3)	0	4571(3)	15(1)
C(4)	3282(3)	0	5451(4)	20(1)
C(5)	3618(2)	-2559(3)	4362(2)	19(1)
C(6)	4143(2)	-1588(3)	2591(2)	16(1)
C(7)	1417(2)	713(3)	867(2)	15(1)
C(8)	1152(2)	1156(3)	1639(2)	15(1)
C(9)	974(2)	0	2103(4)	17(1)
C(10)	1635(2)	1583(3)	172(2)	18(1)
C(11)	1060(2)	2567(3)	1886(2)	19(1)
C(12)	640(3)	0	2904(4)	18(1)
Cl(1)	2870(1)	5000	1936(1)	25(1)
O(1)	734(3)	5000	-286(3)	40(1)

Table 5.3 Bond lengths [Å] and angles [°] for [Cp*RhCp*]Cl · H_2O (**52**)

Rh(1)−C(8)#1	2.183(3)
Rh(1)−C(8)	2.183(3)
Rh(1)−C(1)#1	2.189(2)
Rh(1)−C(1)	2.189(2)
Rh(1)−C(7)#1	2.187(3)
Rh(1)−C(7)	2.187(3)
Rh(1)−C(2)#1	2.193(3)
Rh(1)−C(2)	2.193(3)
Rh(1)−C(3)	2.193(4)
Rh(1)−C(9)	2.197(3)
C(1)−C(1)#1	1.434(5)
C(1)−C(2)	1.448(4)
C(1)−C(6)	1.510(4)
C(2)−C(3)	1.455(4)
C(2)−C(5)	1.494(4)
C(3)−C(2)#1	1.455(4)
C(3)−C(4)	1.494(5)
C(4)−H(4A)	0.98
C(4)−H(4B)	0.98
C(4)−H(4C)	0.98
C(5)−H(5A)	0.98
C(5)−H(5B)	0.98
C(5)−H(5C)	0.98
C(6)−H(6A)	0.98
C(6)−H(6B)	0.98
C(6)−H(6C)	0.98
C(7)−C(7)#1	1.447(5)
C(7)−C(8)	1.446(4)
C(7)−C(10)	1.500(4)
C(8)−C(9)	1.450(4)
C(8)−C(11)	1.501(4)
C(9)−C(8)#1	1.450(4)
C(9)−C(12)	1.506(5)
C(10)−H(10A)	0.98
C(10)−H(10B)	0.98
C(10)−H(10C)	0.98
C(11)−H(11A)	0.98
C(11)−H(11B)	0.98
C(11)−H(11C)	0.98
C(12)−H(12A)	0.98
C(12)−H(12B)	0.98
C(12)−H(12C)	0.98
O(1)−H(1A)	0.980(3)
O(1)−H(1B)	0.979(3)

Table 5.3 continued

C(8)#1−Rh(1)−C(8)	64.97(15)
C(8)#1−Rh(1)−C(1)#1	158.74(10)
C(8)−Rh(1)−C(1)#1	125.45(10)
C(8)#1−Rh(1)−C(1)	125.45(10)
C(8)−Rh(1)−C(1)	158.74(10)
C(1)#1−Rh(1)−C(1)	38.25(14)
C(8)#1−Rh(1)−C(7)#1	38.65(10)
C(8)−Rh(1)−C(7)#1	64.80(10)
C(1)#1−Rh(1)−C(7)#1	124.42(10)
C(1)−Rh(1)−C(7)#1	110.40(10)
C(8)#1−Rh(1)−C(7)	64.80(10)
C(8)−Rh(1)−C(7)	38.65(10)
C(1)#1−Rh(1)−C(7)	110.40(10)
C(1)−Rh(1)−C(7)	124.42(10)
C(7)#1−Rh(1)−C(7)	38.62(14)
C(8)#1−Rh(1)−C(2)#1	161.36(11)
C(8)−Rh(1)−C(2)#1	111.86(10)
C(1)#1−Rh(1)−C(2)#1	38.61(10)
C(1)−Rh(1)−C(2)#1	64.49(10)
C(7)#1−Rh(1)−C(2)#1	158.82(10)
C(7)−Rh(1)−C(2)#1	125.33(10)
C(8)#1−Rh(1)−C(2)	111.86(10)
C(8)−Rh(1)−C(2)	161.36(11)
C(1)#1−Rh(1)−C(2)	64.49(10)
C(1)−Rh(1)−C(2)	38.61(10)
C(7)#1−Rh(1)−C(2)	125.33(10)
C(7)−Rh(1)−C(2)	158.82(10)
C(2)#1−Rh(1)−C(2)	64.76(14)
C(8)#1−Rh(1)−C(3)	126.86(10)
C(8)−Rh(1)−C(3)	126.86(10)
C(1)#1−Rh(1)−C(3)	64.72(11)
C(1)−Rh(1)−C(3)	64.72(11)
C(7)#1−Rh(1)−C(3)	160.30(8)
C(7)−Rh(1)−C(3)	160.30(8)
C(2)#1−Rh(1)−C(3)	38.74(9)
C(2)−Rh(1)−C(3)	38.74(9)
C(8)#1−Rh(1)−C(9)	38.65(9)
C(8)−Rh(1)−C(9)	38.65(9)
C(1)#1−Rh(1)−C(9)	160.53(7)
C(1)−Rh(1)−C(9)	160.53(7)
C(7)#1−Rh(1)−C(9)	64.57(12)
C(7)−Rh(1)−C(9)	64.57(12)
C(2)#1−Rh(1)−C(9)	127.16(11)

Table 5.3 continued

C(2)−Rh(1)−C(9)	127.16(11)
C(3)−Rh(1)−C(9)	113.12(15)
C(1)#1−C(1)−C(2)	108.40(16)
C(1)#1−C(1)−C(6)	126.32(15)
C(2)−C(1)−C(6)	125.3(2)
C(1)#1−C(1)−Rh(1)	70.88(7)
C(2)−C(1)−Rh(1)	70.84(14)
C(6)−C(1)−Rh(1)	124.50(17)
C(1)−C(2)−C(3)	107.8(2)
C(1)−C(2)−C(5)	126.3(2)
C(3)−C(2)−C(5)	125.9(3)
C(1)−C(2)−Rh(1)	70.56(15)
C(3)−C(2)−Rh(1)	70.62(18)
C(5)−C(2)−Rh(1)	125.31(18)
C(2)−C(3)−C(2)#1	107.7(3)
C(2)−C(3)−C(4)	126.16(17)
C(2)#1−C(3)−C(4)	126.16(17)
C(2)−C(3)−Rh(1)	70.64(18)
C(2)#1−C(3)−Rh(1)	70.64(18)
C(4)−C(3)−Rh(1)	125.4(3)
C(3)−C(4)−H(4A)	109.5
C(3)−C(4)−H(4B)	109.5
H(4A)−C(4)−H(4B)	109.5
C(3)−C(4)−H(4C)	109.5
H(4A)−C(4)−H(4C)	109.5
H(4B)−C(4)−H(4C)	109.5
C(2)−C(5)−H(5A)	109.5
C(2)−C(5)−H(5B)	109.5
H(5A)−C(5)−H(5B)	109.5
C(2)−C(5)−H(5C)	109.5
H(5A)−C(5)−H(5C)	109.5
H(5B)−C(5)−H(5C)	109.5
C(1)−C(6)−H(6A)	109.5
C(1)−C(6)−H(6B)	109.5
H(6A)−C(6)−H(6B)	109.5
C(1)−C(6)−H(6C)	109.5
H(6A)−C(6)−H(6C)	109.5
H(6B)−C(6)−H(6C)	109.5
C(7)#1−C(7)−C(8)	108.10(16)
C(7)#1−C(7)−C(10)	126.05(15)
C(8)−C(7)−C(10)	125.8(3)
C(7)#1−C(7)−Rh(1)	70.69(7)
C(8)−C(7)−Rh(1)	70.53(15)
C(10)−C(7)−Rh(1)	125.28(18)

Table 5.3 continued

C(7)−C(8)−C(9)	107.9(2)
C(7)−C(8)−C(11)	125.6(2)
C(9)−C(8)−C(11)	126.5(2)
C(7)−C(8)−Rh(1)	70.82(15)
C(9)−C(8)−Rh(1)	71.20(17)
C(11)−C(8)−Rh(1)	124.62(19)
C(8)#1−C(9)−C(8)	108.0(3)
C(8)#1−C(9)−C(12)	126.02(17)
C(8)−C(9)−C(12)	126.02(17)
C(8)#1−C(9)−Rh(1)	70.15(17)
C(8)−C(9)−Rh(1)	70.15(17)
C(12)−C(9)−Rh(1)	126.3(3)
C(7)−C(10)−H(10A)	109.5
C(7)−C(10)−H(10B)	109.5
H(10A)−C(10)−H(10B)	109.5
C(7)−C(10)−H(10C)	109.5
H(10A)−C(10)−H(10C)	109.5
H(10B)−C(10)−H(10C)	109.5
C(8)−C(11)−H(11A)	109.5
C(8)−C(11)−H(11B)	109.5
H(11A)−C(11)−H(11B)	109.5
C(8)−C(11)−H(11C)	109.5
H(11A)−C(11)−H(11C)	109.5
H(11B)−C(11)−H(11C)	109.5
C(9)−C(12)−H(12A)	109.5
C(9)−C(12)−H(12B)	109.5
H(12A)−C(12)−H(12B)	109.5
C(9)−C(12)−H(12C)	109.5
H(12A)−C(12)−H(12C)	109.5
H(12B)−C(12)−H(12C)	109.5
H(1A)−O(1)−H(1B)	(5)

Symmetry transformations used to generate equivalent atoms: #1 x, $-y$, z

Table 5.4 Anisotropic displacement parameters ($Å^2 \times 10^3$) for [Cp*RhCp*]Cl · H_2O (**52**). The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2\ a^{*2}\ U^{11} + \ldots + 2\ h\ k\ a^*\ b^*\ U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Rh(1)	9(1)	14(1)	9(1)	0	5(1)	0
C(1)	8(1)	18(1)	12(1)	3(1)	5(1)	2(1)
C(2)	8(1)	22(1)	11(1)	1(1)	3(1)	1(1)
C(3)	11(2)	20(2)	10(2)	0	3(2)	0
C(4)	20(2)	32(2)	14(2)	0	13(2)	0
C(5)	17(1)	24(1)	16(1)	5(1)	8(1)	1(1)
C(6)	16(1)	15(1)	19(1)	0(1)	11(1)	2(1)
C(7)	11(1)	19(2)	13(1)	2(1)	6(1)	0(1)
C(8)	8(1)	21(2)	12(1)	3(1)	3(1)	4(1)
C(9)	4(2)	25(2)	16(2)	0	3(1)	0
C(10)	19(1)	20(1)	13(1)	3(1)	8(1)	1(1)
C(11)	18(1)	19(1)	23(2)	-1(1)	12(1)	2(1)
C(12)	18(2)	24(2)	16(2)	0	11(2)	0
Cl(1)	27(1)	20(1)	32(1)	0	20(1)	0
O(1)	34(2)	35(2)	34(2)	0	10(2)	0

Table 5.5 Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($Å^2 \times 10^3$) for [Cp*RhCp*]Cl · H_2O (**52**)

	x	y	z	U(eq)
H(4A)	3877	-27	6248	30
H(4B)	2887	-775	5325	30
H(4C)	2920	802	5356	30
H(5A)	3407	-3114	3676	29
H(5B)	3152	-2629	4567	29
H(5C)	4253	-2852	5029	29
H(6A)	3952	-1146	1858	24
H(6B)	3786	-2417	2406	24
H(6C)	4837	-1774	3058	24
H(10A)	2056	1113	15	27
H(10B)	1958	2386	621	27
H(10C)	1032	1819	-576	27
H(11A)	423	2903	1257	29
H(11B)	1562	3096	1924	29
H(11C)	1134	2624	2640	29
H(12A)	-66	20	2430	27
H(12B)	897	779	3414	27
H(12C)	873	-798	3390	27
H(1A)	1425(11)	5000	350(40)	60
H(1B)	650(40)	5000	350(40)	60

Table 5.6 Torsion angles [°] for [Cp*RhCp*]Cl · H_2O (**52**)

C(8)#1−Rh(1)−C(1)−C(1)#1	160.86(11)
C(8)−Rh(1)−C(1)−C(1)#1	47.4(3)
C(7)#1−Rh(1)−C(1)−C(1)#1	120.16(9)
C(7)−Rh(1)−C(1)−C(1)#1	79.24(10)
C(2)#1−Rh(1)−C(1)−C(1)#1	−37.49(10)
C(2)−Rh(1)−C(1)−C(1)#1	−118.30(14)
C(3)−Rh(1)−C(1)−C(1)#1	−80.57(6)
C(9)−Rh(1)−C(1)−C(1)#1	−168.7(4)
C(8)#1−Rh(1)−C(1)−C(2)	−80.84(18)
C(8)−Rh(1)−C(1)−C(2)	165.7(2)
C(1)#1−Rh(1)−C(1)−C(2)	118.30(14)
C(7)#1−Rh(1)−C(1)−C(2)	−121.54(16)
C(7)−Rh(1)−C(1)−C(2)	−162.46(15)
C(2)#1−Rh(1)−C(1)−C(2)	80.8(2)
C(3)−Rh(1)−C(1)−C(2)	37.73(14)
C(9)−Rh(1)−C(1)−C(2)	−50.4(4)
C(8)#1−Rh(1)−C(1)−C(6)	39.4(3)
C(8)−Rh(1)−C(1)−C(6)	−74.1(4)
C(1)#1−Rh(1)−C(1)−C(6)	−121.5(2)
C(7)#1−Rh(1)−C(1)−C(6)	−1.3(3)
C(7)−Rh(1)−C(1)−C(6)	−42.3(3)
C(2)#1−Rh(1)−C(1)−C(6)	−159.0(3)
C(2)−Rh(1)−C(1)−C(6)	120.2(3)
C(3)−Rh(1)−C(1)−C(6)	157.9(2)
C(9)−Rh(1)−C(1)−C(6)	69.8(4)
C(1)#1−C(1)−C(2)−C(3)	0.1(2)
C(6)−C(1)−C(2)−C(3)	179.6(2)
Rh(1)−C(1)−C(2)−C(3)	−61.1(2)
C(1)#1−C(1)−C(2)−C(5)	−178.7(2)
C(6)−C(1)−C(2)−C(5)	0.8(4)
Rh(1)−C(1)−C(2)−C(5)	120.1(3)
C(1)#1−C(1)−C(2)−Rh(1)	61.24(7)
C(6)−C(1)−C(2)−Rh(1)	−119.3(2)
C(8)#1−Rh(1)−C(2)−C(1)	119.95(16)
C(8)−Rh(1)−C(2)−C(1)	−163.8(3)
C(1)#1−Rh(1)−C(2)−C(1)	−37.15(16)
C(7)#1−Rh(1)−C(2)−C(1)	78.28(18)
C(7)−Rh(1)−C(2)−C(1)	43.5(3)
C(2)#1−Rh(1)−C(2)−C(1)	−80.07(16)
C(3)−Rh(1)−C(2)−C(1)	−117.9(2)
C(9)−Rh(1)−C(2)−C(1)	161.20(15)
C(8)#1−Rh(1)−C(2)−C(3)	−122.20(18)
C(8)−Rh(1)−C(2)−C(3)	−45.9(4)
C(1)#1−Rh(1)−C(2)−C(3)	80.70(18)

Table 5.6 continued

C(1)−Rh(1)−C(2)−C(3)	117.9(2)
C(7)#1−Rh(1)−C(2)−C(3)	−163.87(17)
C(7)−Rh(1)−C(2)−C(3)	161.3(2)
C(2)#1−Rh(1)−C(2)−C(3)	37.79(19)
C(9)−Rh(1)−C(2)−C(3)	−80.9(2)
C(8)#1−Rh(1)−C(2)−C(5)	−1.4(3)
C(8)−Rh(1)−C(2)−C(5)	74.9(4)
C(1)#1−Rh(1)−C(2)−C(5)	−158.4(3)
C(1)−Rh(1)−C(2)−C(5)	−121.3(3)
C(7)#1−Rh(1)−C(2)−C(5)	−43.0(3)
C(7)−Rh(1)−C(2)−C(5)	−77.8(4)
C(2)#1−Rh(1)−C(2)−C(5)	158.63(19)
C(3)−Rh(1)−C(2)−C(5)	120.8(3)
C(9)−Rh(1)−C(2)−C(5)	39.9(3)
C(1)−C(2)−C(3)−C(2)#1	−0.2(4)
C(5)−C(2)−C(3)−C(2)#1	178.61(17)
Rh(1)−C(2)−C(3)−C(2)#1	−61.3(2)
C(1)−C(2)−C(3)−C(4)	−178.7(3)
C(5)−C(2)−C(3)−C(4)	0.1(5)
Rh(1)−C(2)−C(3)−C(4)	120.2(4)
C(1)−C(2)−C(3)−Rh(1)	61.10(19)
C(5)−C(2)−C(3)−Rh(1)	−120.1(3)
C(8)#1−Rh(1)−C(3)−C(2)	79.0(2)
C(8)−Rh(1)−C(3)−C(2)	163.33(16)
C(1)#1−Rh(1)−C(3)−C(2)	−80.08(18)
C(1)−Rh(1)−C(3)−C(2)	−37.60(17)
C(7)#1−Rh(1)−C(3)−C(2)	42.3(4)
C(7)−Rh(1)−C(3)−C(2)	−160.0(3)
C(2)#1−Rh(1)−C(3)−C(2)	−117.7(3)
C(9)−Rh(1)−C(3)−C(2)	121.16(16)
C(8)#1−Rh(1)−C(3)−C(2)#1	−163.33(16)
C(8)−Rh(1)−C(3)−C(2)#1	−79.0(2)
C(1)#1−Rh(1)−C(3)−C(2)#1	37.60(17)
C(1)−Rh(1)−C(3)−C(2)#1	80.08(18)
C(7)#1−Rh(1)−C(3)−C(2)#1	160.0(3)
C(7)−Rh(1)−C(3)−C(2)#1	−42.3(4)
C(2)−Rh(1)−C(3)−C(2)#1	117.7(3)
C(9)−Rh(1)−C(3)−C(2)#1	−121.16(16)
C(8)#1−Rh(1)−C(3)−C(4)	−42.17(10)
C(8)−Rh(1)−C(3)−C(4)	42.17(10)
C(1)#1−Rh(1)−C(3)−C(4)	158.76(8)
C(1)−Rh(1)−C(3)−C(4)	−158.76(8)
C(7)#1−Rh(1)−C(3)−C(4)	−78.9(3)
C(7)−Rh(1)−C(3)−C(4)	78.9(3)

Table 5.6 continued

C(2)#1−Rh(1)−C(3)−C(4)	121.16(16)
C(2)−Rh(1)−C(3)−C(4)	−121.16(16)
C(9)−Rh(1)−C(3)−C(4)	0
C(8)#1−Rh(1)−C(7)−C(7)#1	−37.45(9)
C(8)−Rh(1)−C(7)−C(7)#1	−118.23(14)
C(1)#1−Rh(1)−C(7)−C(7)#1	120.04(9)
C(1)−Rh(1)−C(7)−C(7)#1	79.59(10)
C(2)#1−Rh(1)−C(7)−C(7)#1	160.72(11)
C(2)−Rh(1)−C(7)−C(7)#1	48.2(2)
C(3)−Rh(1)−C(7)−C(7)#1	−168.2(4)
C(9)−Rh(1)−C(7)−C(7)#1	−80.41(6)
C(8)#1−Rh(1)−C(7)−C(8)	80.8(2)
C(1)#1−Rh(1)−C(7)−C(8)	−121.72(16)
C(1)−Rh(1)−C(7)−C(8)	−162.18(15)
C(7)#1−Rh(1)−C(7)−C(8)	118.23(14)
C(2)#1−Rh(1)−C(7)−C(8)	−81.05(18)
C(2)−Rh(1)−C(7)−C(8)	166.5(2)
C(3)−Rh(1)−C(7)−C(8)	−50.0(4)
C(9)−Rh(1)−C(7)−C(8)	37.83(14)
C(8)#1−Rh(1)−C(7)−C(10)	−158.5(3)
C(8)−Rh(1)−C(7)−C(10)	120.7(3)
C(1)#1−Rh(1)−C(7)−C(10)	−1.0(3)
C(1)−Rh(1)−C(7)−C(10)	−41.5(3)
C(7)#1−Rh(1)−C(7)−C(10)	−121.1(2)
C(2)#1−Rh(1)−C(7)−C(10)	39.7(3)
C(2)−Rh(1)−C(7)−C(10)	−72.8(4)
C(3)−Rh(1)−C(7)−C(10)	70.7(4)
C(9)−Rh(1)−C(7)−C(10)	158.5(3)
C(7)#1−C(7)−C(8)−C(9)	−0.9(2)
C(10)−C(7)−C(8)−C(9)	178.1(3)
Rh(1)−C(7)−C(8)−C(9)	−61.9(2)
C(7)#1−C(7)−C(8)−C(11)	−179.6(2)
C(10)−C(7)−C(8)−C(11)	−0.6(4)
Rh(1)−C(7)−C(8)−C(11)	119.4(3)
C(7)#1−C(7)−C(8)−Rh(1)	61.02(7)
C(10)−C(7)−C(8)−Rh(1)	−120.0(3)
C(8)#1−Rh(1)−C(8)−C(7)	−80.30(16)
C(1)#1−Rh(1)−C(8)−C(7)	78.15(18)
C(1)−Rh(1)−C(8)−C(7)	44.1(4)
C(7)#1−Rh(1)−C(8)−C(7)	−37.43(17)
C(2)#1−Rh(1)−C(8)−C(7)	119.74(16)
C(2)−Rh(1)−C(8)−C(7)	−164.6(3)
C(3)−Rh(1)−C(8)−C(7)	161.18(14)
C(9)−Rh(1)−C(8)−C(7)	−117.5(2)

Table 5.6 continued

C(8)#1−Rh(1)−C(8)−C(9)	37.2(2)
C(1)#1−Rh(1)−C(8)−C(9)	−164.30(17)
C(1)−Rh(1)−C(8)−C(9)	161.7(3)
C(7)#1−Rh(1)−C(8)−C(9)	80.12(19)
C(7)−Rh(1)−C(8)−C(9)	117.5(2)
C(2)#1−Rh(1)−C(8)−C(9)	−122.72(18)
C(2)−Rh(1)−C(8)−C(9)	−47.1(4)
C(3)−Rh(1)−C(8)−C(9)	−81.3(2)
C(8)#1−Rh(1)−C(8)−C(11)	159.13(18)
C(1)#1−Rh(1)−C(8)−C(11)	−42.4(3)
C(1)−Rh(1)−C(8)−C(11)	−76.5(4)
C(7)#1−Rh(1)−C(8)−C(11)	−158.0(3)
C(7)−Rh(1)−C(8)−C(11)	−120.6(3)
C(2)#1−Rh(1)−C(8)−C(11)	−0.8(3)
C(2)−Rh(1)−C(8)−C(11)	74.8(4)
C(3)−Rh(1)−C(8)−C(11)	40.6(3)
C(9)−Rh(1)−C(8)−C(11)	121.9(3)
C(7)−C(8)−C(9)−C(8)#1	1.4(4)
C(11)−C(8)−C(9)−C(8)#1	−179.88(17)
Rh(1)−C(8)−C(9)−C(8)#1	−60.2(2)
C(7)−C(8)−C(9)−C(12)	−177.3(3)
C(11)−C(8)−C(9)−C(12)	1.4(5)
Rh(1)−C(8)−C(9)−C(12)	121.0(4)
C(7)−C(8)−C(9)−Rh(1)	61.65(19)
C(11)−C(8)−C(9)−Rh(1)	−119.7(3)
C(8)−Rh(1)−C(9)−C(8)#1	118.6(3)
C(1)#1−Rh(1)−C(9)−C(8)#1	160.0(3)
C(1)−Rh(1)−C(9)−C(8)#1	−41.4(5)
C(7)#1−Rh(1)−C(9)−C(8)#1	37.82(17)
C(7)−Rh(1)−C(9)−C(8)#1	80.78(19)
C(2)#1−Rh(1)−C(9)−C(8)#1	−162.92(16)
C(2)−Rh(1)−C(9)−C(8)#1	−78.5(2)
C(3)−Rh(1)−C(9)−C(8)#1	−120.70(16)
C(8)#1−Rh(1)−C(9)−C(8)	−118.6(3)
C(1)#1−Rh(1)−C(9)−C(8)	41.4(5)
C(1)−Rh(1)−C(9)−C(8)	−160.0(3)
C(7)#1−Rh(1)−C(9)−C(8)	−80.78(19)
C(7)−Rh(1)−C(9)−C(8)	−37.82(17)
C(2)#1−Rh(1)−C(9)−C(8)	78.5(2)
C(2)−Rh(1)−C(9)−C(8)	162.92(16)
C(3)−Rh(1)−C(9)−C(8)	120.70(16)
C(8)#1−Rh(1)−C(9)−C(12)	120.70(16)
C(8)−Rh(1)−C(9)−C(12)	−120.70(16)
C(1)#1−Rh(1)−C(9)−C(12)	−79.3(4)

Table 5.6 continued

C(1)−Rh(1)−C(9)−C(12)	79.3(4)
C(7)#1−Rh(1)−C(9)−C(12)	158.52(8)
C(7)−Rh(1)−C(9)−C(12)	−158.52(8)
C(2)#1−Rh(1)−C(9)−C(12)	−42.22(11)
C(2)−Rh(1)−C(9)−C(12)	42.22(11)
C(3)−Rh(1)−C(9)−C(12)	0

Symmetry transformations used to generate equivalent atoms: #1 x, $-y$, z

Table 5.7 Hydrogen bonds for [Cp*RhCp*]Cl · H_2O (**52**)

D−H···A	d(D−H)	d(H···A)	d(D···A)	<(DHA)
O(1)−H(1A)···Cl(1)	0.980(3)	2.158(13)	3.128(4)	170(6)
O(1)−H(1B)···O(1)#2	0.979(3)	2.28(5)	3.008(8)	130(5)

Symmetry transformations used to generate equivalent atoms: #1 x, $-y$, z; #2 $-x$, $-y+1$, $-z$.

6 Full X-ray data of [Cp*Rh(μ-S_3N_2)-(μ-SSO_3)RhCp*] · CH_2Cl_2

Table 6.1 Crystal data and structure refinement for [Cp*Rh(μ–S_3N_2)(μ–SSO_3)RhCp*] · CH_2Cl_2 (**53**)

Identification code	vmdw12
Empirical formula	C21 H32 Cl2 N2 O3 Rh2 S5
Formula weight	797.51
Temperature	93(2) K
Wavelength	0.710 73 Å
Crystal system	Monoclinic
Space group	P2(1)/c
Unit cell dimensions	a = 10.615(3) Å $\alpha = 90°$
	b = 23.415(6) Å $\beta = 90.089(4)°$
	c = 23.361(6) Å $\gamma = 90°$
Volume	5806(2) Å^3
Z	8
Density (calculated)	1.825 Mg/m^3
Absorption coefficient	1.708 mm^{-1}
F(000)	3200
Crystal size	0.1300 × 0.0100 × 0.0100 mm^3
Theta range for data collection	1.95 to 25.32°
Index ranges	$-12 \leq h \leq 9, -28 \leq k \leq 27, -28 \leq l \leq 25$
Reflections collected	43104
Independent reflections	9933 [R(int) = 0.1725]
Completeness to theta = 25.00°	94.3 %
Absorption correction	Multiscan
Max. and min. transmission	1.0000 and 0.8438
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	9933 / 54 / 649
Goodness-of-fit on F^2	1.13
Final R indices [I>2sigma(I)]	R1 = 0.1107, wR2 = 0.2688
R indices (all data)	R1 = 0.1485, wR2 = 0.2972
Largest diff. peak and hole	3.386 and −2.291 e·Å^{-3}

Table 6.2 Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters (Å$^2 \times 10^3$) for [Cp*Rh(μ−S_3N_2)(μ−SSO_3)RhCp*] · CH_2Cl_2 (**53**). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Rh(1)	5577(1)	3099(1)	4890(1)	19(1)
Rh(2)	2671(1)	3133(1)	5124(1)	19(1)
S(1)	3980(3)	3718(2)	4547(1)	21(1)
N(1)	4157(12)	4344(6)	4898(5)	32(3)
S(2)	4410(4)	4414(2)	5555(2)	31(1)
N(2)	4540(11)	3872(5)	5946(5)	23(3)
S(3)	4426(3)	3184(2)	5753(1)	21(1)
S(4)	3947(3)	2441(2)	4665(1)	21(1)
S(5)	4144(3)	1714(2)	5230(2)	24(1)
O(1)	4479(9)	1928(4)	5779(4)	25(2)
O(2)	2904(10)	1437(5)	5205(4)	31(2)
O(3)	5117(9)	1375(5)	4957(4)	29(2)
C(1)	7292(14)	3610(7)	4757(6)	25(3)
C(2)	7446(14)	3242(7)	5237(6)	26(3)
C(3)	7378(15)	2667(7)	5058(6)	29(4)
C(4)	7136(13)	2675(6)	4449(5)	21(3)
C(5)	7071(13)	3254(6)	4267(5)	19(3)
C(6)	7405(15)	4250(7)	4765(7)	34(4)
C(7)	7759(14)	3439(8)	5840(6)	31(4)
C(8)	7552(14)	2157(7)	5432(6)	27(3)
C(9)	6976(17)	2150(8)	4081(6)	38(4)
C(10)	6872(15)	3474(7)	3660(6)	32(4)
C(11)	1005(13)	3695(7)	5224(6)	24(3)
C(12)	1171(14)	3368(8)	5738(6)	30(4)
C(13)	1072(13)	2772(6)	5592(6)	22(3)
C(14)	823(14)	2740(7)	4972(6)	24(3)
C(15)	804(13)	3317(6)	4761(5)	19(3)
C(16)	1019(15)	4322(7)	5203(6)	28(3)
C(17)	1355(15)	3596(8)	6324(5)	31(4)
C(18)	1132(15)	2269(7)	5998(7)	34(4)
C(19)	614(14)	2202(6)	4638(6)	22(3)
C(20)	584(16)	3451(8)	4145(6)	35(4)
Rh(22)	1562(1)	4933(1)	8206(1)	19(1)
Rh(21)	-1343(1)	5024(1)	7978(1)	19(1)
S(23)	193(3)	5733(2)	8175(1)	21(1)
N(22)	-3(13)	5918(6)	8863(5)	31(3)
S(22)	-300(4)	5526(2)	9385(2)	31(1)
N(21)	-381(12)	4860(6)	9302(5)	29(3)
S(21)	-181(3)	4515(2)	8679(1)	23(1)
S(24)	309(3)	4636(2)	7419(1)	22(1)
S(25)	647(4)	5206(2)	6706(1)	23(1)

Table 6.2 continued

O(21)	1889(9)	5030(5)	6502(4)	27(2)
O(22)	-373(10)	5057(5)	6310(4)	30(3)
O(23)	611(10)	5784(5)	6937(4)	32(3)
C(21)	3049(13)	4887(7)	8868(5)	23(3)
C(22)	3124(12)	4390(6)	8506(5)	18(3)
C(23)	3356(13)	4582(6)	7930(5)	19(3)
C(24)	3430(15)	5203(7)	7935(6)	25(3)
C(25)	3254(13)	5393(6)	8533(5)	19(3)
C(26)	2885(16)	4878(7)	9511(5)	31(4)
C(27)	3022(16)	3776(7)	8701(6)	31(4)
C(28)	3596(16)	4235(7)	7410(6)	32(4)
C(29)	3763(14)	5570(7)	7454(6)	29(4)
C(30)	3251(16)	5971(7)	8733(6)	32(4)
C(31)	-3175(13)	5093(6)	8384(6)	21(3)
C(32)	-3158(14)	4593(7)	8017(6)	28(4)
C(33)	-2935(14)	4767(7)	7458(6)	22(3)
C(34)	-2856(15)	5376(7)	7442(6)	28(3)
C(35)	-3006(13)	5574(7)	8024(6)	27(4)
C(36)	-3471(15)	5097(7)	9015(6)	28(3)
C(37)	-3365(14)	3988(7)	8236(6)	30(4)
C(38)	-2841(16)	4392(8)	6929(6)	35(4)
C(39)	-2747(15)	5768(7)	6933(6)	32(4)
C(40)	-3035(15)	6174(7)	8213(6)	33(4)
C(41)	159(19)	7090(10)	7393(8)	55(5)
Cl(1)	1583(12)	7201(6)	7813(4)	156(4)
Cl(2)	-167(19)	7720(6)	7041(5)	229(9)
C(42)	4560(50)	2570(20)	7075(15)	170(20)
Cl(3)	3180(20)	2510(6)	7597(6)	91(6)
Cl(4)	6230(50)	2458(11)	7211(10)	270(30)
Cl(5)	5704(18)	2895(11)	7199(8)	125(7)
Cl(6)	4100(40)	2409(14)	7751(10)	220(20)

Table 6.3 Bond lengths [Å] and angles [°] for [Cp*Rh(μ−S_3N_2)(μ−SSO_3)RhCp*] · CH_2Cl_2 (**53**)

Rh(1)−C(2)	2.168(14)
Rh(1)−C(5)	2.184(13)
Rh(1)−C(4)	2.190(14)
Rh(1)−C(3)	2.198(16)
Rh(1)−C(1)	2.200(15)
Rh(1)−S(3)	2.367(3)
Rh(1)−S(1)	2.369(4)
Rh(1)−S(4)	2.376(4)
Rh(1)−Rh(2)	3.1347(17)
Rh(2)−C(13)	2.190(14)
Rh(2)−C(14)	2.195(15)
Rh(2)−C(15)	2.197(14)
Rh(2)−C(12)	2.213(15)
Rh(2)−C(11)	2.217(15)
Rh(2)−S(4)	2.370(4)
Rh(2)−S(3)	2.374(4)
Rh(2)−S(1)	2.374(4)
S(1)−N(1)	1.690(14)
N(1)−S(2)	1.566(13)
S(2)−N(2)	1.569(12)
N(2)−S(3)	1.679(13)
S(4)−S(5)	2.163(5)
S(5)−O(1)	1.422(10)
S(5)−O(3)	1.450(11)
S(5)−O(2)	1.469(11)
C(1)−C(2)	1.42(2)
C(1)−C(5)	1.43(2)
C(1)−C(6)	1.50(2)
C(2)−C(3)	1.41(2)
C(2)−C(7)	1.519(18)
C(3)−C(4)	1.447(19)
C(3)−C(8)	1.49(2)
C(4)−C(5)	1.42(2)
C(4)−C(9)	1.51(2)
C(5)−C(10)	1.523(17)
C(6)−H(6A)	0.98
C(6)−H(6B)	0.98
C(6)−H(6C)	0.98
C(7)−H(7A)	0.98
C(7)−H(7B)	0.98
C(7)−H(7C)	0.98
C(8)−H(8A)	0.98
C(8)−H(8B)	0.98
C(8)−H(8C)	0.98

Table 6.3 continued

C(9)−H(9A)	0.98
C(9)−H(9B)	0.98
C(9)−H(9C)	0.98
C(10)−H(10A)	0.98
C(10)−H(10B)	0.98
C(10)−H(10C)	0.98
C(11)−C(15)	1.413(19)
C(11)−C(12)	1.434(19)
C(11)−C(16)	1.47(2)
C(12)−C(13)	1.44(2)
C(12)−C(17)	1.48(2)
C(13)−C(14)	1.473(19)
C(13)−C(18)	1.51(2)
C(14)−C(15)	1.44(2)
C(14)−C(19)	1.497(19)
C(15)−C(20)	1.492(19)
C(16)−H(16A)	0.98
C(16)−H(16B)	0.98
C(16)−H(16C)	0.98
C(17)−H(17A)	0.98
C(17)−H(17B)	0.98
C(17)−H(17C)	0.98
C(18)−H(18A)	0.98
C(18)−H(18B)	0.98
C(18)−H(18C)	0.98
C(19)−H(19A)	0.98
C(19)−H(19B)	0.98
C(19)−H(19C)	0.98
C(20)−H(20A)	0.98
C(20)−H(20B)	0.98
C(20)−H(20C)	0.98
Rh(22)−C(23)	2.173(14)
Rh(22)−C(24)	2.176(16)
Rh(22)−C(22)	2.205(14)
Rh(22)−C(21)	2.211(13)
Rh(22)−C(25)	2.228(14)
Rh(22)−S(21)	2.369(4)
Rh(22)−S(23)	2.370(4)
Rh(22)−S(24)	2.371(3)
Rh(22)−Rh(21)	3.1356(18)
Rh(21)−C(33)	2.165(15)
Rh(21)−C(31)	2.170(14)
Rh(21)−C(32)	2.177(16)
Rh(21)−C(35)	2.188(14)

Table 6.3 continued

Rh(21)−C(34)	2.196(15)
Rh(21)−S(21)	2.370(4)
Rh(21)−S(24)	2.370(4)
Rh(21)−S(23)	2.371(4)
S(23)−N(22)	1.679(12)
N(22)−S(22)	1.559(14)
S(22)−N(21)	1.576(15)
N(21)−S(21)	1.677(13)
S(24)−S(25)	2.163(5)
S(25)−O(23)	1.458(12)
S(25)−O(21)	1.461(11)
S(25)−O(22)	1.464(11)
C(21)−C(25)	1.44(2)
C(21)−C(22)	1.44(2)
C(21)−C(26)	1.514(16)
C(22)−C(23)	1.442(17)
C(22)−C(27)	1.51(2)
C(23)−C(24)	1.45(2)
C(23)−C(28)	1.484(19)
C(24)−C(29)	1.459(19)
C(24)−C(25)	1.478(18)
C(25)−C(30)	1.43(2)
C(26)−H(26A)	0.98
C(26)−H(26B)	0.98
C(26)−H(26C)	0.98
C(27)−H(27A)	0.98
C(27)−H(27B)	0.98
C(27)−H(27C)	0.98
C(28)−H(28A)	0.98
C(28)−H(28B)	0.98
C(28)−H(28C)	0.98
C(29)−H(29A)	0.98
C(29)−H(29B)	0.98
C(29)−H(29C)	0.98
C(30)−H(30A)	0.98
C(30)−H(30B)	0.98
C(30)−H(30C)	0.98
C(31)−C(35)	1.42(2)
C(31)−C(32)	1.45(2)
C(31)−C(36)	1.507(18)
C(32)−C(33)	1.388(19)
C(32)−C(37)	1.52(2)
C(33)−C(34)	1.43(2)
C(33)−C(38)	1.519(19)

Table 6.3 continued

C(34)−C(35)	1.446(19)
C(34)−C(39)	1.51(2)
C(35)−C(40)	1.47(2)
C(36)−H(36A)	0.98
C(36)−H(36B)	0.98
C(36)−H(36C)	0.98
C(37)−H(37A)	0.98
C(37)−H(37B)	0.98
C(37)−H(37C)	0.98
C(38)−H(38A)	0.98
C(38)−H(38B)	0.98
C(38)−H(38C)	0.98
C(39)−H(39A)	0.98
C(39)−H(39B)	0.98
C(39)−H(39C)	0.98
C(40)−H(40A)	0.98
C(40)−H(40B)	0.98
C(40)−H(40C)	0.98
C(41)−Cl(2)	1.72(2)
C(41)−Cl(1)	1.82(2)
C(41)−H(41A)	0.99
C(41)−H(41B)	0.99
Cl(1)−Cl(4)#1	2.40(5)
C(42)−Cl(5)	1.46(5)
C(42)−Cl(6)	1.70(5)
C(42)−Cl(4)	1.82(7)
C(42)−Cl(3)	1.91(5)
Cl(3)−Cl(6)	1.06(4)
Cl(4)−Cl(5)	1.16(3)
Cl(4)−Cl(1)#2	2.40(5)
Cl(5)−Cl(6)	2.42(5)
C(2)−Rh(1)−C(5)	63.8(5)
C(2)−Rh(1)−C(4)	63.5(5)
C(5)−Rh(1)−C(4)	38.0(5)
C(2)−Rh(1)−C(3)	37.7(6)
C(5)−Rh(1)−C(3)	64.1(5)
C(4)−Rh(1)−C(3)	38.5(5)
C(2)−Rh(1)−C(1)	38.0(5)
C(5)−Rh(1)−C(1)	38.2(5)
C(4)−Rh(1)−C(1)	63.5(6)
C(3)−Rh(1)−C(1)	63.6(6)
C(2)−Rh(1)−S(3)	98.2(4)
C(5)−Rh(1)−S(3)	158.4(4)

Table 6.3 continued

C(4)−Rh(1)−S(3)	146.1(4)
C(3)−Rh(1)−S(3)	109.6(4)
C(1)−Rh(1)−S(3)	120.2(4)
C(2)−Rh(1)−S(1)	133.4(4)
C(5)−Rh(1)−S(1)	101.1(4)
C(4)−Rh(1)−S(1)	131.2(4)
C(3)−Rh(1)−S(1)	164.5(4)
C(1)−Rh(1)−S(1)	102.2(4)
S(3)−Rh(1)−S(1)	82.38(12)
C(2)−Rh(1)−S(4)	148.0(4)
C(5)−Rh(1)−S(4)	119.3(4)
C(4)−Rh(1)−S(4)	98.7(4)
C(3)−Rh(1)−S(4)	111.9(5)
C(1)−Rh(1)−S(4)	157.5(4)
S(3)−Rh(1)−S(4)	82.31(12)
S(1)−Rh(1)−S(4)	78.54(13)
C(2)−Rh(1)−Rh(2)	146.2(4)
C(5)−Rh(1)−Rh(2)	145.9(4)
C(4)−Rh(1)−Rh(2)	146.9(4)
C(3)−Rh(1)−Rh(2)	146.7(4)
C(1)−Rh(1)−Rh(2)	145.7(4)
S(3)−Rh(1)−Rh(2)	48.70(9)
S(1)−Rh(1)−Rh(2)	48.69(9)
S(4)−Rh(1)−Rh(2)	48.58(9)
C(13)−Rh(2)−C(14)	39.3(5)
C(13)−Rh(2)−C(15)	64.5(5)
C(14)−Rh(2)−C(15)	38.3(5)
C(13)−Rh(2)−C(12)	38.2(6)
C(14)−Rh(2)−C(12)	64.3(5)
C(15)−Rh(2)−C(12)	63.4(5)
C(13)−Rh(2)−C(11)	63.7(5)
C(14)−Rh(2)−C(11)	63.5(6)
C(15)−Rh(2)−C(11)	37.3(5)
C(12)−Rh(2)−C(11)	37.8(5)
C(13)−Rh(2)−S(4)	114.0(4)
C(14)−Rh(2)−S(4)	98.7(4)
C(15)−Rh(2)−S(4)	118.4(4)
C(12)−Rh(2)−S(4)	151.1(5)
C(11)−Rh(2)−S(4)	155.5(4)
C(13)−Rh(2)−S(3)	108.6(4)
C(14)−Rh(2)−S(3)	145.2(4)
C(15)−Rh(2)−S(3)	159.3(4)
C(12)−Rh(2)−S(3)	98.7(4)
C(11)−Rh(2)−S(3)	122.0(4)

Table 6.3 continued

S(4)−Rh(2)−S(3)	82.30(13)
C(13)−Rh(2)−S(1)	164.0(4)
C(14)−Rh(2)−S(1)	132.4(4)
C(15)−Rh(2)−S(1)	101.3(4)
C(12)−Rh(2)−S(1)	130.3(5)
C(11)−Rh(2)−S(1)	100.7(4)
S(4)−Rh(2)−S(1)	78.57(13)
S(3)−Rh(2)−S(1)	82.13(13)
C(13)−Rh(2)−Rh(1)	147.3(4)
C(14)−Rh(2)−Rh(1)	147.2(4)
C(15)−Rh(2)−Rh(1)	145.6(3)
C(12)−Rh(2)−Rh(1)	145.9(4)
C(11)−Rh(2)−Rh(1)	144.9(4)
S(4)−Rh(2)−Rh(1)	48.74(9)
S(3)−Rh(2)−Rh(1)	48.52(9)
S(1)−Rh(2)−Rh(1)	48.56(9)
N(1)−S(1)−Rh(1)	106.7(5)
N(1)−S(1)−Rh(2)	106.8(5)
Rh(1)−S(1)−Rh(2)	82.75(12)
S(2)−N(1)−S(1)	125.9(8)
N(1)−S(2)−N(2)	120.0(7)
S(2)−N(2)−S(3)	127.9(7)
N(2)−S(3)−Rh(1)	105.8(4)
N(2)−S(3)−Rh(2)	105.7(4)
Rh(1)−S(3)−Rh(2)	82.79(11)
S(5)−S(4)−Rh(2)	108.44(17)
S(5)−S(4)−Rh(1)	107.78(18)
Rh(2)−S(4)−Rh(1)	82.68(12)
O(1)−S(5)−O(3)	114.3(6)
O(1)−S(5)−O(2)	114.3(6)
O(3)−S(5)−O(2)	112.3(6)
O(1)−S(5)−S(4)	107.3(5)
O(3)−S(5)−S(4)	103.4(5)
O(2)−S(5)−S(4)	103.8(5)
C(2)−C(1)−C(5)	107.2(13)
C(2)−C(1)−C(6)	125.8(14)
C(5)−C(1)−C(6)	127.0(13)
C(2)−C(1)−Rh(1)	69.8(8)
C(5)−C(1)−Rh(1)	70.3(8)
C(6)−C(1)−Rh(1)	127.3(10)
C(3)−C(2)−C(1)	109.8(12)
C(3)−C(2)−C(7)	125.1(14)
C(1)−C(2)−C(7)	124.8(15)
C(3)−C(2)−Rh(1)	72.3(9)

Table 6.3 continued

C(1)−C(2)−Rh(1)	72.2(8)
C(7)−C(2)−Rh(1)	126.3(11)
C(2)−C(3)−C(4)	106.8(13)
C(2)−C(3)−C(8)	125.8(13)
C(4)−C(3)−C(8)	127.4(15)
C(2)−C(3)−Rh(1)	70.0(9)
C(4)−C(3)−Rh(1)	70.4(8)
C(8)−C(3)−Rh(1)	125.5(11)
C(5)−C(4)−C(3)	108.3(12)
C(5)−C(4)−C(9)	127.0(13)
C(3)−C(4)−C(9)	124.7(14)
C(5)−C(4)−Rh(1)	70.8(8)
C(3)−C(4)−Rh(1)	71.1(8)
C(9)−C(4)−Rh(1)	123.6(10)
C(4)−C(5)−C(1)	107.9(12)
C(4)−C(5)−C(10)	127.4(13)
C(1)−C(5)−C(10)	124.7(14)
C(4)−C(5)−Rh(1)	71.2(8)
C(1)−C(5)−Rh(1)	71.5(8)
C(10)−C(5)−Rh(1)	125.2(10)
C(1)−C(6)−H(6A)	109.5
C(1)−C(6)−H(6B)	109.5
H(6A)−C(6)−H(6B)	109.5
C(1)−C(6)−H(6C)	109.5
H(6A)−C(6)−H(6C)	109.5
H(6B)−C(6)−H(6C)	109.5
C(2)−C(7)−H(7A)	109.5
C(2)−C(7)−H(7B)	109.5
H(7A)−C(7)−H(7B)	109.5
C(2)−C(7)−H(7C)	109.5
H(7A)−C(7)−H(7C)	109.5
H(7B)−C(7)−H(7C)	109.5
C(3)−C(8)−H(8A)	109.5
C(3)−C(8)−H(8B)	109.5
H(8A)−C(8)−H(8B)	109.5
C(3)−C(8)−H(8C)	109.5
H(8A)−C(8)−H(8C)	109.5
H(8B)−C(8)−H(8C)	109.5
C(4)−C(9)−H(9A)	109.5
C(4)−C(9)−H(9B)	109.5
H(9A)−C(9)−H(9B)	109.5
C(4)−C(9)−H(9C)	109.5
H(9A)−C(9)−H(9C)	109.5
H(9B)−C(9)−H(9C)	109.5

Table 6.3 continued

C(5)−C(10)−H(10A)	109.5
C(5)−C(10)−H(10B)	109.5
H(10A)−C(10)−H(10B)	109.5
C(5)−C(10)−H(10C)	109.5
H(10A)−C(10)−H(10C)	109.5
H(10B)−C(10)−H(10C)	109.5
C(15)−C(11)−C(12)	108.9(14)
C(15)−C(11)−C(16)	127.0(13)
C(12)−C(11)−C(16)	124.0(13)
C(15)−C(11)−Rh(2)	70.5(9)
C(12)−C(11)−Rh(2)	71.0(8)
C(16)−C(11)−Rh(2)	125.6(11)
C(11)−C(12)−C(13)	108.1(13)
C(11)−C(12)−C(17)	126.6(16)
C(13)−C(12)−C(17)	125.2(14)
C(11)−C(12)−Rh(2)	71.3(8)
C(13)−C(12)−Rh(2)	70.0(8)
C(17)−C(12)−Rh(2)	126.5(10)
C(12)−C(13)−C(14)	107.1(12)
C(12)−C(13)−C(18)	127.1(13)
C(14)−C(13)−C(18)	125.6(14)
C(12)−C(13)−Rh(2)	71.8(8)
C(14)−C(13)−Rh(2)	70.5(8)
C(18)−C(13)−Rh(2)	125.5(10)
C(15)−C(14)−C(13)	106.9(12)
C(15)−C(14)−C(19)	127.5(12)
C(13)−C(14)−C(19)	125.5(13)
C(15)−C(14)−Rh(2)	70.9(8)
C(13)−C(14)−Rh(2)	70.2(8)
C(19)−C(14)−Rh(2)	124.6(10)
C(11)−C(15)−C(14)	108.9(12)
C(11)−C(15)−C(20)	129.0(14)
C(14)−C(15)−C(20)	122.1(13)
C(11)−C(15)−Rh(2)	72.1(8)
C(14)−C(15)−Rh(2)	70.8(8)
C(20)−C(15)−Rh(2)	123.6(10)
C(11)−C(16)−H(16A)	109.5
C(11)−C(16)−H(16B)	109.5
H(16A)−C(16)−H(16B)	109.5
C(11)−C(16)−H(16C)	109.5
H(16A)−C(16)−H(16C)	109.5
H(16B)−C(16)−H(16C)	109.5
C(12)−C(17)−H(17A)	109.5
C(12)−C(17)−H(17B)	109.5

Table 6.3 continued

H(17A)−C(17)−H(17B)	109.5
C(12)−C(17)−H(17C)	109.5
H(17A)−C(17)−H(17C)	109.5
H(17B)−C(17)−H(17C)	109.5
C(13)−C(18)−H(18A)	109.5
C(13)−C(18)−H(18B)	109.5
H(18A)−C(18)−H(18B)	109.5
C(13)−C(18)−H(18C)	109.5
H(18A)−C(18)−H(18C)	109.5
H(18B)−C(18)−H(18C)	109.5
C(14)−C(19)−H(19A)	109.5
C(14)−C(19)−H(19B)	109.5
H(19A)−C(19)−H(19B)	109.5
C(14)−C(19)−H(19C)	109.5
H(19A)−C(19)−H(19C)	109.5
H(19B)−C(19)−H(19C)	109.5
C(15)−C(20)−H(20A)	109.5
C(15)−C(20)−H(20B)	109.5
H(20A)−C(20)−H(20B)	109.5
C(15)−C(20)−H(20C)	109.5
H(20A)−C(20)−H(20C)	109.5
H(20B)−C(20)−H(20C)	109.5
C(23)−Rh(22)−C(24)	39.1(5)
C(23)−Rh(22)−C(22)	38.4(4)
C(24)−Rh(22)−C(22)	64.8(5)
C(23)−Rh(22)−C(21)	64.1(5)
C(24)−Rh(22)−C(21)	64.4(5)
C(22)−Rh(22)−C(21)	38.1(5)
C(23)−Rh(22)−C(25)	65.0(5)
C(24)−Rh(22)−C(25)	39.2(5)
C(22)−Rh(22)−C(25)	64.1(5)
C(21)−Rh(22)−C(25)	37.8(5)
C(23)−Rh(22)−S(21)	131.9(4)
C(24)−Rh(22)−S(21)	165.6(4)
C(22)−Rh(22)−S(21)	101.5(4)
C(21)−Rh(22)−S(21)	102.2(4)
C(25)−Rh(22)−S(21)	132.0(3)
C(23)−Rh(22)−S(23)	145.8(4)
C(24)−Rh(22)−S(23)	108.7(4)
C(22)−Rh(22)−S(23)	157.8(4)
C(21)−Rh(22)−S(23)	119.8(4)
C(25)−Rh(22)−S(23)	97.1(4)
S(21)−Rh(22)−S(23)	82.04(13)
C(23)−Rh(22)−S(24)	98.6(4)

Table 6.3 continued

C(24)−Rh(22)−S(24)	111.7(4)
C(22)−Rh(22)−S(24)	119.9(4)
C(21)−Rh(22)−S(24)	157.9(4)
C(25)−Rh(22)−S(24)	149.1(3)
S(21)−Rh(22)−S(24)	78.65(13)
S(23)−Rh(22)−S(24)	82.27(13)
C(23)−Rh(22)−Rh(21)	146.9(4)
C(24)−Rh(22)−Rh(21)	145.8(4)
C(22)−Rh(22)−Rh(21)	146.3(4)
C(21)−Rh(22)−Rh(21)	145.4(3)
C(25)−Rh(22)−Rh(21)	144.9(4)
S(21)−Rh(22)−Rh(21)	48.59(9)
S(23)−Rh(22)−Rh(21)	48.61(9)
S(24)−Rh(22)−Rh(21)	48.59(9)
C(33)−Rh(21)−C(31)	64.4(5)
C(33)−Rh(21)−C(32)	37.3(5)
C(31)−Rh(21)−C(32)	39.0(6)
C(33)−Rh(21)−C(35)	64.0(5)
C(31)−Rh(21)−C(35)	38.0(6)
C(32)−Rh(21)−C(35)	63.7(6)
C(33)−Rh(21)−C(34)	38.2(6)
C(31)−Rh(21)−C(34)	64.3(5)
C(32)−Rh(21)−C(34)	63.3(6)
C(35)−Rh(21)−C(34)	38.5(5)
C(33)−Rh(21)−S(21)	130.7(4)
C(31)−Rh(21)−S(21)	101.6(4)
C(32)−Rh(21)−S(21)	101.4(4)
C(35)−Rh(21)−S(21)	133.0(4)
C(34)−Rh(21)−S(21)	164.2(4)
C(33)−Rh(21)−S(24)	99.3(4)
C(31)−Rh(21)−S(24)	159.0(4)
C(32)−Rh(21)−S(24)	120.0(4)
C(35)−Rh(21)−S(24)	148.2(4)
C(34)−Rh(21)−S(24)	111.7(4)
S(21)−Rh(21)−S(24)	78.65(12)
C(33)−Rh(21)−S(23)	147.1(4)
C(31)−Rh(21)−S(23)	118.7(4)
C(32)−Rh(21)−S(23)	157.7(4)
C(35)−Rh(21)−S(23)	97.7(4)
C(34)−Rh(21)−S(23)	110.5(4)
S(21)−Rh(21)−S(23)	82.00(13)
S(24)−Rh(21)−S(23)	82.27(13)
C(33)−Rh(21)−Rh(22)	147.4(4)
C(31)−Rh(21)−Rh(22)	144.3(4)

Table 6.3 continued

C(32)−Rh(21)−Rh(22)	146.2(4)
C(35)−Rh(21)−Rh(22)	145.6(4)
C(34)−Rh(21)−Rh(22)	147.2(4)
S(21)−Rh(21)−Rh(22)	48.56(9)
S(24)−Rh(21)−Rh(22)	48.61(9)
S(23)−Rh(21)−Rh(22)	48.58(9)
N(22)−S(23)−Rh(22)	104.6(5)
N(22)−S(23)−Rh(21)	106.3(5)
Rh(22)−S(23)−Rh(21)	82.81(13)
S(22)−N(22)−S(23)	128.5(8)
N(22)−S(22)−N(21)	119.9(6)
S(22)−N(21)−S(21)	125.2(8)
N(21)−S(21)−Rh(22)	107.8(5)
N(21)−S(21)−Rh(21)	106.9(5)
Rh(22)−S(21)−Rh(21)	82.85(12)
S(25)−S(24)−Rh(21)	108.17(19)
S(25)−S(24)−Rh(22)	108.83(18)
Rh(21)−S(24)−Rh(22)	82.80(11)
O(23)−S(25)−O(21)	113.9(6)
O(23)−S(25)−O(22)	115.8(6)
O(21)−S(25)−O(22)	113.2(6)
O(23)−S(25)−S(24)	106.4(4)
O(21)−S(25)−S(24)	103.2(5)
O(22)−S(25)−S(24)	102.5(5)
C(25)−C(21)−C(22)	109.8(11)
C(25)−C(21)−C(26)	124.8(14)
C(22)−C(21)−C(26)	125.2(14)
C(25)−C(21)−Rh(22)	71.8(8)
C(22)−C(21)−Rh(22)	70.7(7)
C(26)−C(21)−Rh(22)	127.7(10)
C(21)−C(22)−C(23)	107.7(12)
C(21)−C(22)−C(27)	126.1(12)
C(23)−C(22)−C(27)	126.2(13)
C(21)−C(22)−Rh(22)	71.2(8)
C(23)−C(22)−Rh(22)	69.6(8)
C(27)−C(22)−Rh(22)	126.2(10)
C(22)−C(23)−C(24)	108.4(12)
C(22)−C(23)−C(28)	128.5(14)
C(24)−C(23)−C(28)	123.0(12)
C(22)−C(23)−Rh(22)	72.0(8)
C(24)−C(23)−Rh(22)	70.6(8)
C(28)−C(23)−Rh(22)	126.9(10)
C(23)−C(24)−C(29)	126.6(13)
C(23)−C(24)−C(25)	107.5(12)

Table 6.3 continued

C(29)−C(24)−C(25)	125.6(14)
C(23)−C(24)−Rh(22)	70.3(8)
C(29)−C(24)−Rh(22)	128.1(11)
C(25)−C(24)−Rh(22)	72.3(8)
C(30)−C(25)−C(21)	126.9(12)
C(30)−C(25)−C(24)	126.4(13)
C(21)−C(25)−C(24)	106.6(12)
C(30)−C(25)−Rh(22)	124.5(11)
C(21)−C(25)−Rh(22)	70.5(8)
C(24)−C(25)−Rh(22)	68.5(8)
C(21)−C(26)−H(26A)	109.5
C(21)−C(26)−H(26B)	109.5
H(26A)−C(26)−H(26B)	109.5
C(21)−C(26)−H(26C)	109.5
H(26A)−C(26)−H(26C)	109.5
H(26B)−C(26)−H(26C)	109.5
C(22)−C(27)−H(27A)	109.5
C(22)−C(27)−H(27B)	109.5
H(27A)−C(27)−H(27B)	109.5
C(22)−C(27)−H(27C)	109.5
H(27A)−C(27)−H(27C)	109.5
H(27B)−C(27)−H(27C)	109.5
C(23)−C(28)−H(28A)	109.5
C(23)−C(28)−H(28B)	109.5
H(28A)−C(28)−H(28B)	109.5
C(23)−C(28)−H(28C)	109.5
H(28A)−C(28)−H(28C)	109.5
H(28B)−C(28)−H(28C)	109.5
C(24)−C(29)−H(29A)	109.5
C(24)−C(29)−H(29B)	109.5
H(29A)−C(29)−H(29B)	109.5
C(24)−C(29)−H(29C)	109.5
H(29A)−C(29)−H(29C)	109.5
H(29B)−C(29)−H(29C)	109.5
C(25)−C(30)−H(30A)	109.5
C(25)−C(30)−H(30B)	109.5
H(30A)−C(30)−H(30B)	109.5
C(25)−C(30)−H(30C)	109.5
H(30A)−C(30)−H(30C)	109.5
H(30B)−C(30)−H(30C)	109.5
C(35)−C(31)−C(32)	106.7(11)
C(35)−C(31)−C(36)	127.1(13)
C(32)−C(31)−C(36)	125.8(13)
C(35)−C(31)−Rh(21)	71.7(8)

Table 6.3 continued

C(32)−C(31)−Rh(21)	70.7(8)
C(36)−C(31)−Rh(21)	128.0(11)
C(33)−C(32)−C(31)	108.7(14)
C(33)−C(32)−C(37)	128.0(15)
C(31)−C(32)−C(37)	123.3(12)
C(33)−C(32)−Rh(21)	70.9(9)
C(31)−C(32)−Rh(21)	70.2(8)
C(37)−C(32)−Rh(21)	125.0(11)
C(32)−C(33)−C(34)	109.2(13)
C(32)−C(33)−C(38)	127.3(15)
C(34)−C(33)−C(38)	123.4(13)
C(32)−C(33)−Rh(21)	71.8(9)
C(34)−C(33)−Rh(21)	72.1(8)
C(38)−C(33)−Rh(21)	124.4(10)
C(33)−C(34)−C(35)	106.8(13)
C(33)−C(34)−C(39)	129.3(13)
C(35)−C(34)−C(39)	123.7(15)
C(33)−C(34)−Rh(21)	69.7(8)
C(35)−C(34)−Rh(21)	70.4(8)
C(39)−C(34)−Rh(21)	128.5(11)
C(31)−C(35)−C(34)	108.5(13)
C(31)−C(35)−C(40)	125.2(13)
C(34)−C(35)−C(40)	126.2(15)
C(31)−C(35)−Rh(21)	70.4(8)
C(34)−C(35)−Rh(21)	71.1(8)
C(40)−C(35)−Rh(21)	126.4(11)
C(31)−C(36)−H(36A)	109.5
C(31)−C(36)−H(36B)	109.5
H(36A)−C(36)−H(36B)	109.5
C(31)−C(36)−H(36C)	109.5
H(36A)−C(36)−H(36C)	109.5
H(36B)−C(36)−H(36C)	109.5
C(32)−C(37)−H(37A)	109.5
C(32)−C(37)−H(37B)	109.5
H(37A)−C(37)−H(37B)	109.5
C(32)−C(37)−H(37C)	109.5
H(37A)−C(37)−H(37C)	109.5
H(37B)−C(37)−H(37C)	109.5
C(33)−C(38)−H(38A)	109.5
C(33)−C(38)−H(38B)	109.5
H(38A)−C(38)−H(38B)	109.5
C(33)−C(38)−H(38C)	109.5
H(38A)−C(38)−H(38C)	109.5
H(38B)−C(38)−H(38C)	109.5

Table 6.3 continued

C(34)−C(39)−H(39A)	109.5
C(34)−C(39)−H(39B)	109.5
H(39A)−C(39)−H(39B)	109.5
C(34)−C(39)−H(39C)	109.5
H(39A)−C(39)−H(39C)	109.5
H(39B)−C(39)−H(39C)	109.5
C(35)−C(40)−H(40A)	109.5
C(35)−C(40)−H(40B)	109.5
H(40A)−C(40)−H(40B)	109.5
C(35)−C(40)−H(40C)	109.5
H(40A)−C(40)−H(40C)	109.5
H(40B)−C(40)−H(40C)	109.5
Cl(2)−C(41)−Cl(1)	107.6(14)
Cl(2)−C(41)−H(41A)	110.2
Cl(1)−C(41)−H(41A)	110.2
Cl(2)−C(41)−H(41B)	110.2
Cl(1)−C(41)−H(41B)	110.2
H(41A)−C(41)−H(41B)	108.5
C(41)−Cl(1)−Cl(4)#1	145.8(10)
Cl(5)−C(42)−Cl(6)	(3)
Cl(5)−C(42)−Cl(4)	39.8(18)
Cl(6)−C(42)−Cl(4)	(3)
Cl(5)−C(42)−Cl(3)	(3)
Cl(6)−C(42)−Cl(3)	33.6(15)
Cl(4)−C(42)−Cl(3)	(3)
Cl(6)−Cl(3)−C(42)	(3)
Cl(5)−Cl(4)−C(42)	(3)
Cl(5)−Cl(4)−Cl(1)#2	(4)
C(42)−Cl(4)−Cl(1)#2	167.3(19)
Cl(4)−Cl(5)−C(42)	(4)
Cl(4)−Cl(5)−Cl(6)	(3)
C(42)−Cl(5)−Cl(6)	43.6(17)
Cl(3)−Cl(6)−C(42)	(3)
Cl(3)−Cl(6)−Cl(5)	(2)
C(42)−Cl(6)−Cl(5)	36.3(17)

Symmetry transformations used to generate equivalent atoms: #1 $-x+1$, $y+1/2$, $-z+3/2$; #2 $-x+1$, $y-1/2$, $-z+3/2$.

Table 6.4 Anisotropic displacement parameters (Å$^2\times10^3$) for [Cp*Rh(μ−S_3N_2)(μ−SSO_3)RhCp*] · CH_2Cl_2 (**53**).
The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2\ a^{*2}\ U^{11} + \ldots + 2\ h\ k\ a^*\ b^*\ U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Rh(1)	15(1)	23(1)	20(1)	2(1)	2(1)	0(1)
Rh(2)	14(1)	23(1)	20(1)	0(1)	-1(1)	1(1)
S(1)	18(2)	21(2)	25(2)	6(1)	1(1)	2(2)
N(1)	27(8)	29(8)	41(7)	5(6)	-4(6)	-1(6)
S(2)	24(2)	23(2)	45(2)	-4(2)	3(2)	1(2)
N(2)	19(7)	28(7)	23(6)	0(5)	-1(5)	-1(5)
S(3)	11(2)	29(2)	23(2)	-2(1)	-2(1)	0(2)
S(4)	14(2)	24(2)	26(2)	-2(1)	2(1)	2(2)
S(5)	19(2)	24(2)	28(2)	3(1)	-1(1)	-1(2)
O(1)	24(6)	26(6)	24(5)	4(4)	-4(4)	10(4)
O(2)	23(6)	22(6)	48(6)	4(5)	5(5)	0(5)
O(3)	21(6)	30(6)	37(6)	3(5)	-8(4)	2(5)
C(1)	16(8)	22(8)	37(8)	3(6)	8(6)	1(6)
C(2)	12(8)	34(9)	30(7)	-6(6)	-13(6)	-2(7)
C(3)	27(10)	36(10)	25(7)	9(6)	-4(6)	5(7)
C(4)	15(5)	25(5)	23(4)	-8(4)	-1(4)	2(4)
C(5)	12(5)	25(5)	21(4)	2(4)	4(4)	1(4)
C(6)	11(9)	47(11)	45(9)	-18(8)	-8(6)	-1(7)
C(7)	18(9)	47(11)	28(7)	-13(7)	-4(6)	-14(7)
C(8)	19(9)	30(9)	31(7)	5(6)	1(6)	5(7)
C(9)	40(11)	45(11)	30(8)	-17(7)	3(7)	9(8)
C(10)	29(10)	41(10)	26(7)	19(7)	-1(6)	-5(7)
C(11)	14(8)	35(9)	22(6)	3(6)	-5(5)	-1(7)
C(12)	11(9)	55(11)	25(7)	5(7)	-3(6)	5(7)
C(13)	14(8)	21(8)	30(7)	0(6)	6(6)	2(6)
C(14)	20(5)	29(5)	24(4)	-4(4)	1(4)	-4(4)
C(15)	18(8)	17(7)	22(6)	-4(5)	8(5)	-4(6)
C(16)	27(9)	30(9)	27(7)	-2(6)	2(6)	11(7)
C(17)	24(9)	50(11)	21(7)	8(7)	9(6)	16(8)
C(18)	26(10)	33(10)	43(9)	9(7)	9(7)	-9(7)
C(19)	21(4)	22(4)	22(3)	-1(2)	-2(2)	-1(2)
C(20)	36(11)	39(10)	30(8)	-2(7)	-5(7)	-6(8)
Rh(22)	13(1)	25(1)	17(1)	0(1)	0(1)	1(1)
Rh(21)	13(1)	27(1)	17(1)	-1(1)	-1(1)	0(1)
S(23)	20(2)	21(2)	23(2)	1(1)	0(1)	1(2)
N(22)	36(9)	24(7)	34(7)	-10(6)	-1(6)	4(6)
S(22)	25(2)	44(3)	23(2)	-4(2)	1(1)	6(2)
N(21)	15(8)	49(9)	24(6)	5(6)	4(5)	3(6)
S(21)	16(2)	33(2)	21(2)	4(1)	3(1)	1(2)
S(24)	18(2)	29(2)	17(2)	-2(1)	0(1)	0(2)

Table 6.4 continued

S(25)	17(2)	32(2)	19(2)	1(1)	-1(1)	-1(2)
O(21)	18(6)	46(7)	17(5)	-5(4)	-1(4)	-2(5)
O(22)	17(6)	53(8)	21(5)	1(5)	1(4)	3(5)
O(23)	32(7)	37(7)	26(5)	18(5)	-4(4)	-2(5)
C(21)	7(8)	52(11)	11(6)	0(6)	1(5)	1(7)
C(22)	9(5)	21(5)	23(4)	2(4)	5(4)	-2(4)
C(23)	9(8)	29(8)	19(6)	4(6)	-6(5)	-1(6)
C(24)	30(10)	25(8)	19(6)	-5(6)	-1(6)	-1(7)
C(25)	14(5)	25(5)	19(4)	3(4)	-1(4)	0(4)
C(26)	38(11)	43(10)	11(6)	14(6)	-7(6)	-2(8)
C(27)	33(10)	25(9)	34(8)	2(6)	-3(7)	6(7)
C(28)	33(10)	27(9)	36(8)	-3(7)	3(7)	11(7)
C(29)	11(9)	35(9)	41(8)	15(7)	-7(6)	-5(7)
C(30)	32(10)	33(10)	32(8)	-10(7)	-8(6)	1(7)
C(31)	11(8)	32(9)	21(6)	5(6)	8(5)	-4(6)
C(32)	21(9)	41(10)	23(7)	7(6)	2(6)	-4(7)
C(33)	16(5)	26(5)	26(4)	0(4)	3(4)	-3(4)
C(34)	27(5)	30(5)	26(5)	-1(4)	-10(4)	3(4)
C(35)	9(8)	35(9)	37(8)	-21(7)	-2(6)	8(7)
C(36)	27(4)	30(4)	28(4)	0(2)	2(2)	1(2)
C(37)	17(9)	40(10)	34(8)	11(7)	11(6)	-1(7)
C(38)	40(11)	48(11)	16(7)	-13(7)	-14(6)	9(8)
C(39)	21(9)	39(10)	36(8)	8(7)	3(6)	-9(7)
C(40)	23(9)	34(10)	40(8)	0(7)	-4(6)	25(7)
C(41)	45(13)	70(15)	52(11)	2(10)	3(9)	10(11)
Cl(1)	165(10)	180(12)	123(7)	-44(8)	-2(7)	-44(9)
Cl(2)	440(30)	144(12)	102(7)	-23(7)	-69(11)	91(14)
C(42)	250(60)	190(50)	80(20)	0(30)	-20(30)	-120(40)
Cl(3)	171(17)	45(8)	57(8)	-8(6)	28(9)	-42(10)
Cl(4)	620(80)	92(17)	105(16)	-52(14)	-90(30)	90(30)
Cl(5)	109(14)	160(20)	102(12)	-59(13)	-24(10)	-23(13)
Cl(6)	410(60)	150(30)	90(15)	-40(15)	-60(20)	60(30)

Table 6.5 Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters (Å$^2 \times 10^3$) for [Cp*Rh(μ−S_3N_2)(μ−SSO_3)RhCp*] · CH_2Cl_2 (**53**)

	x	y	z	U(eq)
H(6A)	8283	4359	4694	51
H(6B)	7142	4395	5140	51
H(6C)	6865	4413	4467	51
H(7A)	8675	3468	5884	47
H(7B)	7427	3163	6117	47
H(7C)	7376	3814	5908	47
H(8A)	8442	2047	5436	40
H(8B)	7044	1840	5284	40
H(8C)	7282	2249	5823	40
H(9A)	7796	2034	3928	58
H(9B)	6401	2235	3764	58
H(9C)	6626	1839	4313	58
H(10A)	7687	3504	3466	48
H(10B)	6472	3852	3674	48
H(10C)	6327	3209	3450	48
H(16A)	162	4468	5259	42
H(16B)	1335	4448	4830	42
H(16C)	1569	4469	5507	42
H(17A)	532	3661	6502	47
H(17B)	1818	3957	6304	47
H(17C)	1835	3320	6552	47
H(18A)	291	2194	6153	51
H(18B)	1714	2355	6312	51
H(18C)	1430	1931	5791	51
H(19A)	-287	2112	4632	33
H(19B)	1077	1888	4819	33
H(19C)	916	2255	4245	33
H(20A)	-316	3518	4080	53
H(20B)	866	3130	3909	53
H(20C)	1059	3795	4040	53
H(26A)	3713	4855	9696	46
H(26B)	2381	4544	9620	46
H(26C)	2455	5227	9634	46
H(27A)	3857	3635	8811	46
H(27B)	2688	3542	8388	46
H(27C)	2453	3753	9030	46
H(28A)	4492	4137	7391	48
H(28B)	3359	4455	7069	48
H(28C)	3093	3884	7427	48
H(29A)	4680	5616	7439	43
H(29B)	3366	5945	7502	43
H(29C)	3468	5396	7096	43

Table 6.5 continued

H(30A)	4103	6077	8854	49
H(30B)	2672	6005	9057	49
H(30C)	2975	6224	8423	49
H(36A)	-4384	5129	9069	43
H(36B)	-3052	5423	9197	43
H(36C)	-3170	4741	9189	43
H(37A)	-4261	3892	8208	45
H(37B)	-3093	3964	8636	45
H(37C)	-2874	3720	8004	45
H(38A)	-3682	4337	6765	52
H(38B)	-2485	4021	7035	52
H(38C)	-2295	4577	6646	52
H(39A)	-3589	5848	6780	48
H(39B)	-2235	5584	6637	48
H(39C)	-2348	6126	7051	48
H(40A)	-3901	6318	8191	49
H(40B)	-2492	6404	7964	49
H(40C)	-2732	6199	8608	49
H(41A)	287	6778	7114	67
H(41B)	-551	6986	7647	67

Table 6.6 Torsion angles [°] for [Cp*Rh(μ−S_3N_2)(μ−SSO_3)RhCp*] · CH_2Cl_2 (**53**)

C(2)−Rh(1)−Rh(2)−C(13)	−67.1(10)
C(5)−Rh(1)−Rh(2)−C(13)	150.6(10)
C(4)−Rh(1)−Rh(2)−C(13)	78.6(10)
C(3)−Rh(1)−Rh(2)−C(13)	4.5(10)
C(1)−Rh(1)−Rh(2)−C(13)	−138.2(10)
S(3)−Rh(1)−Rh(2)−C(13)	−53.9(7)
S(1)−Rh(1)−Rh(2)−C(13)	−176.4(7)
S(4)−Rh(1)−Rh(2)−C(13)	68.6(7)
C(2)−Rh(1)−Rh(2)−C(14)	−143.9(10)
C(5)−Rh(1)−Rh(2)−C(14)	73.9(10)
C(4)−Rh(1)−Rh(2)−C(14)	1.9(10)
C(3)−Rh(1)−Rh(2)−C(14)	−72.3(11)
C(1)−Rh(1)−Rh(2)−C(14)	145.0(10)
S(3)−Rh(1)−Rh(2)−C(14)	−130.7(7)
S(1)−Rh(1)−Rh(2)−C(14)	106.8(7)
S(4)−Rh(1)−Rh(2)−C(14)	−8.2(7)
C(2)−Rh(1)−Rh(2)−C(15)	143.6(10)
C(5)−Rh(1)−Rh(2)−C(15)	1.3(9)
C(4)−Rh(1)−Rh(2)−C(15)	−70.7(9)
C(3)−Rh(1)−Rh(2)−C(15)	−144.8(10)
C(1)−Rh(1)−Rh(2)−C(15)	72.4(9)
S(3)−Rh(1)−Rh(2)−C(15)	156.8(7)
S(1)−Rh(1)−Rh(2)−C(15)	34.3(7)
S(4)−Rh(1)−Rh(2)−C(15)	−80.7(7)
C(2)−Rh(1)−Rh(2)−C(12)	5.7(11)
C(5)−Rh(1)−Rh(2)−C(12)	−136.6(11)
C(4)−Rh(1)−Rh(2)−C(12)	151.5(11)
C(3)−Rh(1)−Rh(2)−C(12)	77.3(11)
C(1)−Rh(1)−Rh(2)−C(12)	−65.4(10)
S(3)−Rh(1)−Rh(2)−C(12)	18.9(8)
S(1)−Rh(1)−Rh(2)−C(12)	−103.6(8)
S(4)−Rh(1)−Rh(2)−C(12)	141.4(8)
C(2)−Rh(1)−Rh(2)−C(11)	75.2(10)
C(5)−Rh(1)−Rh(2)−C(11)	−67.0(9)
C(4)−Rh(1)−Rh(2)−C(11)	−139.0(9)
C(3)−Rh(1)−Rh(2)−C(11)	146.8(10)
C(1)−Rh(1)−Rh(2)−C(11)	4.1(9)
S(3)−Rh(1)−Rh(2)−C(11)	88.4(6)
S(1)−Rh(1)−Rh(2)−C(11)	−34.1(6)
S(4)−Rh(1)−Rh(2)−C(11)	−149.1(6)
C(2)−Rh(1)−Rh(2)−S(4)	−135.7(8)
C(5)−Rh(1)−Rh(2)−S(4)	82.0(7)
C(4)−Rh(1)−Rh(2)−S(4)	10.0(7)
C(3)−Rh(1)−Rh(2)−S(4)	−64.1(8)

Table 6.6 continued

C(1)−Rh(1)−Rh(2)−S(4)	153.2(7)
S(3)−Rh(1)−Rh(2)−S(4)	−122.52(17)
S(1)−Rh(1)−Rh(2)−S(4)	115.00(17)
C(2)−Rh(1)−Rh(2)−S(3)	−13.2(8)
C(5)−Rh(1)−Rh(2)−S(3)	−155.5(7)
C(4)−Rh(1)−Rh(2)−S(3)	132.6(7)
C(3)−Rh(1)−Rh(2)−S(3)	58.4(8)
C(1)−Rh(1)−Rh(2)−S(3)	−84.3(7)
S(1)−Rh(1)−Rh(2)−S(3)	−122.48(17)
S(4)−Rh(1)−Rh(2)−S(3)	122.52(17)
C(2)−Rh(1)−Rh(2)−S(1)	109.3(8)
C(5)−Rh(1)−Rh(2)−S(1)	−33.0(7)
C(4)−Rh(1)−Rh(2)−S(1)	−105.0(7)
C(3)−Rh(1)−Rh(2)−S(1)	−179.1(8)
C(1)−Rh(1)−Rh(2)−S(1)	38.2(7)
S(3)−Rh(1)−Rh(2)−S(1)	122.48(17)
S(4)−Rh(1)−Rh(2)−S(1)	−115.00(17)
C(2)−Rh(1)−S(1)−N(1)	−28.4(7)
C(5)−Rh(1)−S(1)−N(1)	−92.7(6)
C(4)−Rh(1)−S(1)−N(1)	−119.1(7)
C(3)−Rh(1)−S(1)−N(1)	−76.4(17)
C(1)−Rh(1)−S(1)−N(1)	−53.7(6)
S(3)−Rh(1)−S(1)−N(1)	65.7(5)
S(4)−Rh(1)−S(1)−N(1)	149.3(5)
Rh(2)−Rh(1)−S(1)−N(1)	105.4(5)
C(2)−Rh(1)−S(1)−Rh(2)	−133.8(5)
C(5)−Rh(1)−S(1)−Rh(2)	161.9(4)
C(4)−Rh(1)−S(1)−Rh(2)	135.5(5)
C(3)−Rh(1)−S(1)−Rh(2)	178.2(16)
C(1)−Rh(1)−S(1)−Rh(2)	−159.1(4)
S(3)−Rh(1)−S(1)−Rh(2)	−39.74(12)
S(4)−Rh(1)−S(1)−Rh(2)	43.90(11)
C(13)−Rh(2)−S(1)−N(1)	67.6(15)
C(14)−Rh(2)−S(1)−N(1)	119.3(7)
C(15)−Rh(2)−S(1)−N(1)	93.7(6)
C(12)−Rh(2)−S(1)−N(1)	29.1(7)
C(11)−Rh(2)−S(1)−N(1)	55.6(6)
S(4)−Rh(2)−S(1)−N(1)	−149.3(5)
S(3)−Rh(2)−S(1)−N(1)	−65.6(5)
Rh(1)−Rh(2)−S(1)−N(1)	−105.3(5)
C(13)−Rh(2)−S(1)−Rh(1)	172.9(14)
C(14)−Rh(2)−S(1)−Rh(1)	−135.4(5)
C(15)−Rh(2)−S(1)−Rh(1)	−161.1(4)
C(12)−Rh(2)−S(1)−Rh(1)	134.4(5)

Table 6.6 continued

C(11)−Rh(2)−S(1)−Rh(1)	160.9(4)
S(4)−Rh(2)−S(1)−Rh(1)	−44.04(11)
S(3)−Rh(2)−S(1)−Rh(1)	39.64(12)
Rh(1)−S(1)−N(1)−S(2)	−44.1(10)
Rh(2)−S(1)−N(1)−S(2)	43.2(10)
S(1)−N(1)−S(2)−N(2)	0.9(13)
N(1)−S(2)−N(2)−S(3)	−0.8(13)
S(2)−N(2)−S(3)−Rh(1)	43.7(10)
S(2)−N(2)−S(3)−Rh(2)	−43.1(10)
C(2)−Rh(1)−S(3)−N(2)	68.3(6)
C(5)−Rh(1)−S(3)−N(2)	36.3(12)
C(4)−Rh(1)−S(3)−N(2)	121.8(8)
C(3)−Rh(1)−S(3)−N(2)	105.4(6)
C(1)−Rh(1)−S(3)−N(2)	35.1(6)
S(1)−Rh(1)−S(3)−N(2)	−64.6(4)
S(4)−Rh(1)−S(3)−N(2)	−144.0(4)
Rh(2)−Rh(1)−S(3)−N(2)	−104.4(5)
C(2)−Rh(1)−S(3)−Rh(2)	172.6(4)
C(5)−Rh(1)−S(3)−Rh(2)	140.7(10)
C(4)−Rh(1)−S(3)−Rh(2)	−133.8(7)
C(3)−Rh(1)−S(3)−Rh(2)	−150.3(5)
C(1)−Rh(1)−S(3)−Rh(2)	139.5(5)
S(1)−Rh(1)−S(3)−Rh(2)	39.74(12)
S(4)−Rh(1)−S(3)−Rh(2)	−39.65(12)
C(13)−Rh(2)−S(3)−N(2)	−103.0(6)
C(14)−Rh(2)−S(3)−N(2)	−121.6(8)
C(15)−Rh(2)−S(3)−N(2)	−36.4(11)
C(12)−Rh(2)−S(3)−N(2)	−65.0(6)
C(11)−Rh(2)−S(3)−N(2)	−33.0(6)
S(4)−Rh(2)−S(3)−N(2)	144.2(4)
S(1)−Rh(2)−S(3)−N(2)	64.7(4)
Rh(1)−Rh(2)−S(3)−N(2)	104.4(4)
C(13)−Rh(2)−S(3)−Rh(1)	152.5(4)
C(14)−Rh(2)−S(3)−Rh(1)	134.0(7)
C(15)−Rh(2)−S(3)−Rh(1)	−140.8(10)
C(12)−Rh(2)−S(3)−Rh(1)	−169.4(5)
C(11)−Rh(2)−S(3)−Rh(1)	−137.4(4)
S(4)−Rh(2)−S(3)−Rh(1)	39.77(12)
S(1)−Rh(2)−S(3)−Rh(1)	−39.67(12)
C(13)−Rh(2)−S(4)−S(5)	−40.2(5)
C(14)−Rh(2)−S(4)−S(5)	−78.1(4)
C(15)−Rh(2)−S(4)−S(5)	−113.0(4)
C(12)−Rh(2)−S(4)−S(5)	−27.3(8)
C(11)−Rh(2)−S(4)−S(5)	−119.1(9)

Table 6.6 continued

S(3)−Rh(2)−S(4)−S(5)	66.76(19)
S(1)−Rh(2)−S(4)−S(5)	150.2(2)
Rh(1)−Rh(2)−S(4)−S(5)	106.4(2)
C(13)−Rh(2)−S(4)−Rh(1)	−146.6(4)
C(14)−Rh(2)−S(4)−Rh(1)	175.5(4)
C(15)−Rh(2)−S(4)−Rh(1)	140.6(4)
C(12)−Rh(2)−S(4)−Rh(1)	−133.6(8)
C(11)−Rh(2)−S(4)−Rh(1)	134.5(9)
S(3)−Rh(2)−S(4)−Rh(1)	−39.60(11)
S(1)−Rh(2)−S(4)−Rh(1)	43.88(11)
C(2)−Rh(1)−S(4)−S(5)	25.8(8)
C(5)−Rh(1)−S(4)−S(5)	112.5(5)
C(4)−Rh(1)−S(4)−S(5)	78.4(4)
C(3)−Rh(1)−S(4)−S(5)	40.8(4)
C(1)−Rh(1)−S(4)−S(5)	114.6(11)
S(3)−Rh(1)−S(4)−S(5)	−67.35(18)
S(1)−Rh(1)−S(4)−S(5)	−151.08(19)
Rh(2)−Rh(1)−S(4)−S(5)	−107.08(19)
C(2)−Rh(1)−S(4)−Rh(2)	132.9(8)
C(5)−Rh(1)−S(4)−Rh(2)	−140.4(4)
C(4)−Rh(1)−S(4)−Rh(2)	−174.5(4)
C(3)−Rh(1)−S(4)−Rh(2)	147.9(4)
C(1)−Rh(1)−S(4)−Rh(2)	−138.3(11)
S(3)−Rh(1)−S(4)−Rh(2)	39.73(11)
S(1)−Rh(1)−S(4)−Rh(2)	−44.00(11)
Rh(2)−S(4)−S(5)−O(1)	−48.4(5)
Rh(1)−S(4)−S(5)−O(1)	39.7(5)
Rh(2)−S(4)−S(5)−O(3)	−169.6(4)
Rh(1)−S(4)−S(5)−O(3)	−81.5(5)
Rh(2)−S(4)−S(5)−O(2)	73.0(5)
Rh(1)−S(4)−S(5)−O(2)	161.1(5)
C(5)−Rh(1)−C(1)−C(2)	−117.8(13)
C(4)−Rh(1)−C(1)−C(2)	−80.1(9)
C(3)−Rh(1)−C(1)−C(2)	−36.9(8)
S(3)−Rh(1)−C(1)−C(2)	61.5(9)
S(1)−Rh(1)−C(1)−C(2)	149.7(8)
S(4)−Rh(1)−C(1)−C(2)	−120.7(11)
Rh(2)−Rh(1)−C(1)−C(2)	121.4(9)
C(2)−Rh(1)−C(1)−C(5)	117.8(13)
C(4)−Rh(1)−C(1)−C(5)	37.7(8)
C(3)−Rh(1)−C(1)−C(5)	80.9(9)
S(3)−Rh(1)−C(1)−C(5)	179.3(7)
S(1)−Rh(1)−C(1)−C(5)	−92.5(8)
S(4)−Rh(1)−C(1)−C(5)	−2.9(16)

Table 6.6 continued

Rh(2)−Rh(1)−C(1)−C(5)	−120.8(8)
C(2)−Rh(1)−C(1)−C(6)	−120.2(16)
C(5)−Rh(1)−C(1)−C(6)	122.0(17)
C(4)−Rh(1)−C(1)−C(6)	159.7(15)
C(3)−Rh(1)−C(1)−C(6)	−157.1(15)
S(3)−Rh(1)−C(1)−C(6)	−58.7(14)
S(1)−Rh(1)−C(1)−C(6)	29.5(13)
S(4)−Rh(1)−C(1)−C(6)	119.1(13)
Rh(2)−Rh(1)−C(1)−C(6)	1.2(17)
C(5)−C(1)−C(2)−C(3)	2.3(17)
C(6)−C(1)−C(2)−C(3)	−175.0(14)
Rh(1)−C(1)−C(2)−C(3)	63.0(11)
C(5)−C(1)−C(2)−C(7)	177.1(14)
C(6)−C(1)−C(2)−C(7)	(2)
Rh(1)−C(1)−C(2)−C(7)	−122.3(15)
C(5)−C(1)−C(2)−Rh(1)	−60.6(10)
C(6)−C(1)−C(2)−Rh(1)	122.0(15)
C(5)−Rh(1)−C(2)−C(3)	−80.9(9)
C(4)−Rh(1)−C(2)−C(3)	−38.3(8)
C(1)−Rh(1)−C(2)−C(3)	−118.4(12)
S(3)−Rh(1)−C(2)−C(3)	111.7(8)
S(1)−Rh(1)−C(2)−C(3)	−161.1(7)
S(4)−Rh(1)−C(2)−C(3)	23.1(13)
Rh(2)−Rh(1)−C(2)−C(3)	121.6(8)
C(5)−Rh(1)−C(2)−C(1)	37.6(8)
C(4)−Rh(1)−C(2)−C(1)	80.1(9)
C(3)−Rh(1)−C(2)−C(1)	118.4(12)
S(3)−Rh(1)−C(2)−C(1)	−129.9(8)
S(1)−Rh(1)−C(2)−C(1)	−42.7(10)
S(4)−Rh(1)−C(2)−C(1)	141.5(8)
Rh(2)−Rh(1)−C(2)−C(1)	−119.9(8)
C(5)−Rh(1)−C(2)−C(7)	158.1(16)
C(4)−Rh(1)−C(2)−C(7)	−159.3(16)
C(3)−Rh(1)−C(2)−C(7)	−121.0(18)
C(1)−Rh(1)−C(2)−C(7)	120.5(18)
S(3)−Rh(1)−C(2)−C(7)	−9.4(14)
S(1)−Rh(1)−C(2)−C(7)	77.9(15)
S(4)−Rh(1)−C(2)−C(7)	−97.9(15)
Rh(2)−Rh(1)−C(2)−C(7)	0.6(19)
C(1)−C(2)−C(3)−C(4)	−1.7(17)
C(7)−C(2)−C(3)−C(4)	−176.4(14)
Rh(1)−C(2)−C(3)−C(4)	61.2(10)
C(1)−C(2)−C(3)−C(8)	177.2(14)
C(7)−C(2)−C(3)−C(8)	(3)

Table 6.6 continued

Rh(1)−C(2)−C(3)−C(8)	−119.9(16)
C(1)−C(2)−C(3)−Rh(1)	−62.9(10)
C(7)−C(2)−C(3)−Rh(1)	122.4(15)
C(5)−Rh(1)−C(3)−C(2)	80.0(9)
C(4)−Rh(1)−C(3)−C(2)	117.1(13)
C(1)−Rh(1)−C(3)−C(2)	37.2(8)
S(3)−Rh(1)−C(3)−C(2)	−77.6(9)
S(1)−Rh(1)−C(3)−C(2)	62.1(19)
S(4)−Rh(1)−C(3)−C(2)	−167.1(8)
Rh(2)−Rh(1)−C(3)−C(2)	−120.4(9)
C(2)−Rh(1)−C(3)−C(4)	−117.1(13)
C(5)−Rh(1)−C(3)−C(4)	−37.1(8)
C(1)−Rh(1)−C(3)−C(4)	−79.9(9)
S(3)−Rh(1)−C(3)−C(4)	165.3(8)
S(1)−Rh(1)−C(3)−C(4)	(2)
S(4)−Rh(1)−C(3)−C(4)	75.9(9)
Rh(2)−Rh(1)−C(3)−C(4)	122.5(8)
C(2)−Rh(1)−C(3)−C(8)	120.3(17)
C(5)−Rh(1)−C(3)−C(8)	−159.7(15)
C(4)−Rh(1)−C(3)−C(8)	−122.6(18)
C(1)−Rh(1)−C(3)−C(8)	157.5(15)
S(3)−Rh(1)−C(3)−C(8)	42.7(14)
S(1)−Rh(1)−C(3)−C(8)	−177.6(9)
S(4)−Rh(1)−C(3)−C(8)	−46.7(14)
Rh(2)−Rh(1)−C(3)−C(8)	−0.1(18)
C(2)−C(3)−C(4)−C(5)	0.4(17)
C(8)−C(3)−C(4)−C(5)	−178.4(15)
Rh(1)−C(3)−C(4)−C(5)	61.3(10)
C(2)−C(3)−C(4)−C(9)	−179.2(14)
C(8)−C(3)−C(4)−C(9)	(2)
Rh(1)−C(3)−C(4)−C(9)	−118.3(15)
C(2)−C(3)−C(4)−Rh(1)	−60.9(11)
C(8)−C(3)−C(4)−Rh(1)	120.2(16)
C(2)−Rh(1)−C(4)−C(5)	−80.6(9)
C(3)−Rh(1)−C(4)−C(5)	−118.1(12)
C(1)−Rh(1)−C(4)−C(5)	−37.9(8)
S(3)−Rh(1)−C(4)−C(5)	−143.4(7)
S(1)−Rh(1)−C(4)−C(5)	45.1(9)
S(4)−Rh(1)−C(4)−C(5)	127.4(7)
Rh(2)−Rh(1)−C(4)−C(5)	119.8(8)
C(2)−Rh(1)−C(4)−C(3)	37.5(9)
C(5)−Rh(1)−C(4)−C(3)	118.1(12)
C(1)−Rh(1)−C(4)−C(3)	80.1(9)
S(3)−Rh(1)−C(4)−C(3)	−25.3(13)

Table 6.6 continued

S(1)−Rh(1)−C(4)−C(3)	163.1(7)
S(4)−Rh(1)−C(4)−C(3)	−114.5(9)
Rh(2)−Rh(1)−C(4)−C(3)	−122.1(9)
C(2)−Rh(1)−C(4)−C(9)	157.1(14)
C(5)−Rh(1)−C(4)−C(9)	−122.3(15)
C(3)−Rh(1)−C(4)−C(9)	119.7(16)
C(1)−Rh(1)−C(4)−C(9)	−160.2(14)
S(3)−Rh(1)−C(4)−C(9)	94.3(13)
S(1)−Rh(1)−C(4)−C(9)	−77.2(13)
S(4)−Rh(1)−C(4)−C(9)	5.2(13)
Rh(2)−Rh(1)−C(4)−C(9)	−2.4(17)
C(3)−C(4)−C(5)−C(1)	1.0(16)
C(9)−C(4)−C(5)−C(1)	−179.4(14)
Rh(1)−C(4)−C(5)−C(1)	62.5(10)
C(3)−C(4)−C(5)−C(10)	178.0(14)
C(9)−C(4)−C(5)−C(10)	(2)
Rh(1)−C(4)−C(5)−C(10)	−120.4(15)
C(3)−C(4)−C(5)−Rh(1)	−61.5(10)
C(9)−C(4)−C(5)−Rh(1)	118.1(15)
C(2)−C(1)−C(5)−C(4)	−2.0(16)
C(6)−C(1)−C(5)−C(4)	175.3(14)
Rh(1)−C(1)−C(5)−C(4)	−62.3(10)
C(2)−C(1)−C(5)−C(10)	−179.2(13)
C(6)−C(1)−C(5)−C(10)	(2)
Rh(1)−C(1)−C(5)−C(10)	120.5(14)
C(2)−C(1)−C(5)−Rh(1)	60.3(10)
C(6)−C(1)−C(5)−Rh(1)	−122.4(15)
C(2)−Rh(1)−C(5)−C(4)	79.8(9)
C(3)−Rh(1)−C(5)−C(4)	37.6(8)
C(1)−Rh(1)−C(5)−C(4)	117.1(12)
S(3)−Rh(1)−C(5)−C(4)	115.5(11)
S(1)−Rh(1)−C(5)−C(4)	−147.1(7)
S(4)−Rh(1)−C(5)−C(4)	−64.1(8)
Rh(2)−Rh(1)−C(5)−C(4)	−122.5(8)
C(2)−Rh(1)−C(5)−C(1)	−37.4(9)
C(4)−Rh(1)−C(5)−C(1)	−117.1(12)
C(3)−Rh(1)−C(5)−C(1)	−79.5(9)
S(3)−Rh(1)−C(5)−C(1)	−1.7(16)
S(1)−Rh(1)−C(5)−C(1)	95.7(8)
S(4)−Rh(1)−C(5)−C(1)	178.7(7)
Rh(2)−Rh(1)−C(5)−C(1)	120.4(8)
C(2)−Rh(1)−C(5)−C(10)	−157.2(15)
C(4)−Rh(1)−C(5)−C(10)	123.0(16)
C(3)−Rh(1)−C(5)−C(10)	160.6(15)

Table 6.6 continued

C(1)−Rh(1)−C(5)−C(10)	−119.9(17)
S(3)−Rh(1)−C(5)−C(10)	−121.5(12)
S(1)−Rh(1)−C(5)−C(10)	−24.1(13)
S(4)−Rh(1)−C(5)−C(10)	58.9(14)
Rh(2)−Rh(1)−C(5)−C(10)	0.5(17)
C(13)−Rh(2)−C(11)−C(15)	−81.6(9)
C(14)−Rh(2)−C(11)−C(15)	−37.6(8)
C(12)−Rh(2)−C(11)−C(15)	−119.1(13)
S(4)−Rh(2)−C(11)−C(15)	8.9(15)
S(3)−Rh(2)−C(11)−C(15)	−178.0(6)
S(1)−Rh(2)−C(11)−C(15)	94.7(8)
Rh(1)−Rh(2)−C(11)−C(15)	120.0(8)
C(13)−Rh(2)−C(11)−C(12)	37.4(9)
C(14)−Rh(2)−C(11)−C(12)	81.5(10)
C(15)−Rh(2)−C(11)−C(12)	119.1(13)
S(4)−Rh(2)−C(11)−C(12)	128.0(10)
S(3)−Rh(2)−C(11)−C(12)	−58.9(10)
S(1)−Rh(2)−C(11)−C(12)	−146.2(9)
Rh(1)−Rh(2)−C(11)−C(12)	−121.0(9)
C(13)−Rh(2)−C(11)−C(16)	156.2(13)
C(14)−Rh(2)−C(11)−C(16)	−159.8(13)
C(15)−Rh(2)−C(11)−C(16)	−122.2(15)
C(12)−Rh(2)−C(11)−C(16)	118.8(16)
S(4)−Rh(2)−C(11)−C(16)	−113.3(12)
S(3)−Rh(2)−C(11)−C(16)	59.9(12)
S(1)−Rh(2)−C(11)−C(16)	−27.5(12)
Rh(1)−Rh(2)−C(11)−C(16)	−2.2(15)
C(15)−C(11)−C(12)−C(13)	0.0(17)
C(16)−C(11)−C(12)−C(13)	178.7(14)
Rh(2)−C(11)−C(12)−C(13)	−60.6(10)
C(15)−C(11)−C(12)−C(17)	−177.4(14)
C(16)−C(11)−C(12)−C(17)	(2)
Rh(2)−C(11)−C(12)−C(17)	122.0(15)
C(15)−C(11)−C(12)−Rh(2)	60.6(10)
C(16)−C(11)−C(12)−Rh(2)	−120.6(14)
C(13)−Rh(2)−C(12)−C(11)	−118.2(12)
C(14)−Rh(2)−C(12)−C(11)	−79.2(9)
C(15)−Rh(2)−C(12)−C(11)	−36.4(8)
S(4)−Rh(2)−C(12)−C(11)	−137.5(8)
S(3)−Rh(2)−C(12)−C(11)	132.7(8)
S(1)−Rh(2)−C(12)−C(11)	45.7(10)
Rh(1)−Rh(2)−C(12)−C(11)	118.5(8)
C(14)−Rh(2)−C(12)−C(13)	39.0(8)
C(15)−Rh(2)−C(12)−C(13)	81.8(9)

Table 6.6 continued

C(11)−Rh(2)−C(12)−C(13)	118.2(12)
S(4)−Rh(2)−C(12)−C(13)	−19.3(13)
S(3)−Rh(2)−C(12)−C(13)	−109.1(8)
S(1)−Rh(2)−C(12)−C(13)	163.9(7)
Rh(1)−Rh(2)−C(12)−C(13)	−123.3(8)
C(13)−Rh(2)−C(12)−C(17)	119.6(18)
C(14)−Rh(2)−C(12)−C(17)	158.6(17)
C(15)−Rh(2)−C(12)−C(17)	−158.6(17)
C(11)−Rh(2)−C(12)−C(17)	−122.2(19)
S(4)−Rh(2)−C(12)−C(17)	100.3(16)
S(3)−Rh(2)−C(12)−C(17)	10.6(15)
S(1)−Rh(2)−C(12)−C(17)	−76.5(15)
Rh(1)−Rh(2)−C(12)−C(17)	(2)
C(11)−C(12)−C(13)−C(14)	−0.7(16)
C(17)−C(12)−C(13)−C(14)	176.8(14)
Rh(2)−C(12)−C(13)−C(14)	−62.1(9)
C(11)−C(12)−C(13)−C(18)	−177.4(14)
C(17)−C(12)−C(13)−C(18)	(2)
Rh(2)−C(12)−C(13)−C(18)	121.2(15)
C(11)−C(12)−C(13)−Rh(2)	61.4(10)
C(17)−C(12)−C(13)−Rh(2)	−121.2(15)
C(14)−Rh(2)−C(13)−C(12)	−116.4(12)
C(15)−Rh(2)−C(13)−C(12)	−78.7(8)
C(11)−Rh(2)−C(13)−C(12)	−37.0(8)
S(4)−Rh(2)−C(13)−C(12)	169.9(7)
S(3)−Rh(2)−C(13)−C(12)	80.2(8)
S(1)−Rh(2)−C(13)−C(12)	−50.2(18)
Rh(1)−Rh(2)−C(13)−C(12)	119.9(8)
C(15)−Rh(2)−C(13)−C(14)	37.7(8)
C(12)−Rh(2)−C(13)−C(14)	116.4(12)
C(11)−Rh(2)−C(13)−C(14)	79.4(9)
S(4)−Rh(2)−C(13)−C(14)	−73.6(9)
S(3)−Rh(2)−C(13)−C(14)	−163.3(7)
S(1)−Rh(2)−C(13)−C(14)	66.3(17)
Rh(1)−Rh(2)−C(13)−C(14)	−123.6(8)
C(14)−Rh(2)−C(13)−C(18)	120.5(16)
C(15)−Rh(2)−C(13)−C(18)	158.2(14)
C(12)−Rh(2)−C(13)−C(18)	−123.1(16)
C(11)−Rh(2)−C(13)−C(18)	−160.1(14)
S(4)−Rh(2)−C(13)−C(18)	46.9(13)
S(3)−Rh(2)−C(13)−C(18)	−42.8(13)
S(1)−Rh(2)−C(13)−C(18)	−173.3(10)
Rh(1)−Rh(2)−C(13)−C(18)	−3.1(17)
C(12)−C(13)−C(14)−C(15)	1.1(15)

Table 6.6 continued

C(18)−C(13)−C(14)−C(15)	177.8(13)
Rh(2)−C(13)−C(14)−C(15)	−61.8(9)
C(12)−C(13)−C(14)−C(19)	−178.1(14)
C(18)−C(13)−C(14)−C(19)	(2)
Rh(2)−C(13)−C(14)−C(19)	119.0(14)
C(12)−C(13)−C(14)−Rh(2)	62.9(10)
C(18)−C(13)−C(14)−Rh(2)	−120.3(14)
C(13)−Rh(2)−C(14)−C(15)	116.9(11)
C(12)−Rh(2)−C(14)−C(15)	78.9(8)
C(11)−Rh(2)−C(14)−C(15)	36.7(7)
S(4)−Rh(2)−C(14)−C(15)	−125.6(7)
S(3)−Rh(2)−C(14)−C(15)	145.4(6)
S(1)−Rh(2)−C(14)−C(15)	−43.2(9)
Rh(1)−Rh(2)−C(14)−C(15)	−119.4(8)
C(15)−Rh(2)−C(14)−C(13)	−116.9(11)
C(12)−Rh(2)−C(14)−C(13)	−37.9(8)
C(11)−Rh(2)−C(14)−C(13)	−80.2(9)
S(4)−Rh(2)−C(14)−C(13)	117.5(8)
S(3)−Rh(2)−C(14)−C(13)	28.5(12)
S(1)−Rh(2)−C(14)−C(13)	−160.1(6)
Rh(1)−Rh(2)−C(14)−C(13)	123.7(8)
C(13)−Rh(2)−C(14)−C(19)	−120.1(16)
C(15)−Rh(2)−C(14)−C(19)	123.0(15)
C(12)−Rh(2)−C(14)−C(19)	−158.0(14)
C(11)−Rh(2)−C(14)−C(19)	159.7(13)
S(4)−Rh(2)−C(14)−C(19)	−2.6(12)
S(3)−Rh(2)−C(14)−C(19)	−91.6(12)
S(1)−Rh(2)−C(14)−C(19)	79.8(13)
Rh(1)−Rh(2)−C(14)−C(19)	3.6(16)
C(12)−C(11)−C(15)−C(14)	0.7(17)
C(16)−C(11)−C(15)−C(14)	−178.0(14)
Rh(2)−C(11)−C(15)−C(14)	61.6(10)
C(12)−C(11)−C(15)−C(20)	180.0(14)
C(16)−C(11)−C(15)−C(20)	(3)
Rh(2)−C(11)−C(15)−C(20)	−119.2(15)
C(12)−C(11)−C(15)−Rh(2)	−60.9(10)
C(16)−C(11)−C(15)−Rh(2)	120.4(15)
C(13)−C(14)−C(15)−C(11)	−1.1(16)
C(19)−C(14)−C(15)−C(11)	178.0(14)
Rh(2)−C(14)−C(15)−C(11)	−62.4(10)
C(13)−C(14)−C(15)−C(20)	179.6(13)
C(19)−C(14)−C(15)−C(20)	(2)
Rh(2)−C(14)−C(15)−C(20)	118.3(13)
C(13)−C(14)−C(15)−Rh(2)	61.3(9)

Table 6.6 continued

C(19)−C(14)−C(15)−Rh(2)	−119.5(15)
C(13)−Rh(2)−C(15)−C(11)	79.5(9)
C(14)−Rh(2)−C(15)−C(11)	118.2(11)
C(12)−Rh(2)−C(15)−C(11)	36.8(9)
S(4)−Rh(2)−C(15)−C(11)	−175.8(7)
S(3)−Rh(2)−C(15)−C(11)	4.9(15)
S(1)−Rh(2)−C(15)−C(11)	−92.8(8)
Rh(1)−Rh(2)−C(15)−C(11)	−118.3(8)
C(13)−Rh(2)−C(15)−C(14)	−38.7(8)
C(12)−Rh(2)−C(15)−C(14)	−81.4(9)
C(11)−Rh(2)−C(15)−C(14)	−118.2(11)
S(4)−Rh(2)−C(15)−C(14)	66.0(8)
S(3)−Rh(2)−C(15)−C(14)	−113.4(11)
S(1)−Rh(2)−C(15)−C(14)	149.0(7)
Rh(1)−Rh(2)−C(15)−C(14)	123.5(7)
C(13)−Rh(2)−C(15)−C(20)	−155.1(14)
C(14)−Rh(2)−C(15)−C(20)	−116.3(15)
C(12)−Rh(2)−C(15)−C(20)	162.3(15)
C(11)−Rh(2)−C(15)−C(20)	125.5(16)
S(4)−Rh(2)−C(15)−C(20)	−50.4(13)
S(3)−Rh(2)−C(15)−C(20)	130.3(11)
S(1)−Rh(2)−C(15)−C(20)	32.6(13)
Rh(1)−Rh(2)−C(15)−C(20)	7.1(16)
C(23)−Rh(22)−Rh(21)−C(33)	2.5(10)
C(24)−Rh(22)−Rh(21)−C(33)	76.8(10)
C(22)−Rh(22)−Rh(21)−C(33)	−71.0(9)
C(21)−Rh(22)−Rh(21)−C(33)	−142.1(10)
C(25)−Rh(22)−Rh(21)−C(33)	149.1(9)
S(21)−Rh(22)−Rh(21)−C(33)	−103.6(7)
S(23)−Rh(22)−Rh(21)−C(33)	134.3(7)
S(24)−Rh(22)−Rh(21)−C(33)	11.7(7)
C(23)−Rh(22)−Rh(21)−C(31)	145.7(10)
C(24)−Rh(22)−Rh(21)−C(31)	−140.0(10)
C(22)−Rh(22)−Rh(21)−C(31)	72.2(9)
C(21)−Rh(22)−Rh(21)−C(31)	1.2(10)
C(25)−Rh(22)−Rh(21)−C(31)	−67.7(9)
S(21)−Rh(22)−Rh(21)−C(31)	39.7(7)
S(23)−Rh(22)−Rh(21)−C(31)	−82.4(7)
S(24)−Rh(22)−Rh(21)−C(31)	155.0(7)
C(23)−Rh(22)−Rh(21)−C(32)	73.9(10)
C(24)−Rh(22)−Rh(21)−C(32)	148.2(10)
C(22)−Rh(22)−Rh(21)−C(32)	0.4(9)
C(21)−Rh(22)−Rh(21)−C(32)	−70.6(10)
C(25)−Rh(22)−Rh(21)−C(32)	−139.5(9)

Table 6.6 continued

S(21)−Rh(22)−Rh(21)−C(32)	−32.1(7)
S(23)−Rh(22)−Rh(21)−C(32)	−154.2(7)
S(24)−Rh(22)−Rh(21)−C(32)	83.2(7)
C(23)−Rh(22)−Rh(21)−C(35)	−145.3(10)
C(24)−Rh(22)−Rh(21)−C(35)	−70.9(10)
C(22)−Rh(22)−Rh(21)−C(35)	141.2(10)
C(21)−Rh(22)−Rh(21)−C(35)	70.2(11)
C(25)−Rh(22)−Rh(21)−C(35)	1.3(9)
S(21)−Rh(22)−Rh(21)−C(35)	108.7(8)
S(23)−Rh(22)−Rh(21)−C(35)	−13.4(7)
S(24)−Rh(22)−Rh(21)−C(35)	−136.0(8)
C(23)−Rh(22)−Rh(21)−C(34)	−72.2(10)
C(24)−Rh(22)−Rh(21)−C(34)	2.2(10)
C(22)−Rh(22)−Rh(21)−C(34)	−145.7(10)
C(21)−Rh(22)−Rh(21)−C(34)	143.3(11)
C(25)−Rh(22)−Rh(21)−C(34)	74.4(9)
S(21)−Rh(22)−Rh(21)−C(34)	−178.2(8)
S(23)−Rh(22)−Rh(21)−C(34)	59.7(7)
S(24)−Rh(22)−Rh(21)−C(34)	−62.9(8)
C(23)−Rh(22)−Rh(21)−S(21)	106.1(7)
C(24)−Rh(22)−Rh(21)−S(21)	−179.6(7)
C(22)−Rh(22)−Rh(21)−S(21)	32.6(6)
C(21)−Rh(22)−Rh(21)−S(21)	−38.4(8)
C(25)−Rh(22)−Rh(21)−S(21)	−107.3(6)
S(23)−Rh(22)−Rh(21)−S(21)	−122.09(16)
S(24)−Rh(22)−Rh(21)−S(21)	115.34(18)
C(23)−Rh(22)−Rh(21)−S(24)	−9.3(7)
C(24)−Rh(22)−Rh(21)−S(24)	65.0(7)
C(22)−Rh(22)−Rh(21)−S(24)	−82.8(6)
C(21)−Rh(22)−Rh(21)−S(24)	−153.8(8)
C(25)−Rh(22)−Rh(21)−S(24)	137.3(6)
S(21)−Rh(22)−Rh(21)−S(24)	−115.34(18)
S(23)−Rh(22)−Rh(21)−S(24)	122.57(16)
C(23)−Rh(22)−Rh(21)−S(23)	−131.8(7)
C(24)−Rh(22)−Rh(21)−S(23)	−57.5(7)
C(22)−Rh(22)−Rh(21)−S(23)	154.7(6)
C(21)−Rh(22)−Rh(21)−S(23)	83.6(8)
C(25)−Rh(22)−Rh(21)−S(23)	14.8(6)
S(21)−Rh(22)−Rh(21)−S(23)	122.09(16)
S(24)−Rh(22)−Rh(21)−S(23)	−122.57(16)
C(23)−Rh(22)−S(23)−N(22)	−121.3(8)
C(24)−Rh(22)−S(23)−N(22)	−105.0(6)
C(22)−Rh(22)−S(23)−N(22)	−36.0(11)
C(21)−Rh(22)−S(23)−N(22)	−34.4(7)

Table 6.6 continued

C(25)−Rh(22)−S(23)−N(22)	−66.5(6)
S(21)−Rh(22)−S(23)−N(22)	65.1(5)
S(24)−Rh(22)−S(23)−N(22)	144.7(5)
Rh(21)−Rh(22)−S(23)−N(22)	105.0(5)
C(23)−Rh(22)−S(23)−Rh(21)	133.6(6)
C(24)−Rh(22)−S(23)−Rh(21)	150.0(4)
C(22)−Rh(22)−S(23)−Rh(21)	−141.0(9)
C(21)−Rh(22)−S(23)−Rh(21)	−139.4(4)
C(25)−Rh(22)−S(23)−Rh(21)	−171.5(3)
S(21)−Rh(22)−S(23)−Rh(21)	−39.91(11)
S(24)−Rh(22)−S(23)−Rh(21)	39.63(11)
C(33)−Rh(21)−S(23)−N(22)	122.0(8)
C(31)−Rh(21)−S(23)−N(22)	35.6(7)
C(32)−Rh(21)−S(23)−N(22)	37.2(12)
C(35)−Rh(21)−S(23)−N(22)	69.2(6)
C(34)−Rh(21)−S(23)−N(22)	106.8(7)
S(21)−Rh(21)−S(23)−N(22)	−63.3(5)
S(24)−Rh(21)−S(23)−N(22)	−142.9(5)
Rh(22)−Rh(21)−S(23)−N(22)	−103.2(5)
C(33)−Rh(21)−S(23)−Rh(22)	−134.8(7)
C(31)−Rh(21)−S(23)−Rh(22)	138.8(4)
C(32)−Rh(21)−S(23)−Rh(22)	140.4(10)
C(35)−Rh(21)−S(23)−Rh(22)	172.4(4)
C(34)−Rh(21)−S(23)−Rh(22)	−150.0(4)
S(21)−Rh(21)−S(23)−Rh(22)	39.89(11)
S(24)−Rh(21)−S(23)−Rh(22)	−39.65(11)
Rh(22)−S(23)−N(22)−S(22)	−46.6(11)
Rh(21)−S(23)−N(22)−S(22)	40.1(11)
S(23)−N(22)−S(22)−N(21)	3.3(14)
N(22)−S(22)−N(21)−S(21)	−0.5(13)
S(22)−N(21)−S(21)−Rh(22)	42.8(10)
S(22)−N(21)−S(21)−Rh(21)	−45.0(10)
C(23)−Rh(22)−S(21)−N(21)	119.3(7)
C(24)−Rh(22)−S(21)−N(21)	73.6(16)
C(22)−Rh(22)−S(21)−N(21)	92.2(6)
C(21)−Rh(22)−S(21)−N(21)	53.3(7)
C(25)−Rh(22)−S(21)−N(21)	26.8(7)
S(23)−Rh(22)−S(21)−N(21)	−65.6(5)
S(24)−Rh(22)−S(21)−N(21)	−149.3(5)
Rh(21)−Rh(22)−S(21)−N(21)	−105.5(5)
C(23)−Rh(22)−S(21)−Rh(21)	−135.2(5)
C(24)−Rh(22)−S(21)−Rh(21)	179.1(15)
C(22)−Rh(22)−S(21)−Rh(21)	−162.3(4)
C(21)−Rh(22)−S(21)−Rh(21)	158.8(4)

Table 6.6 continued

C(25)−Rh(22)−S(21)−Rh(21)	132.3(5)
S(23)−Rh(22)−S(21)−Rh(21)	39.92(11)
S(24)−Rh(22)−S(21)−Rh(21)	−43.74(12)
C(33)−Rh(21)−S(21)−N(21)	−117.2(7)
C(31)−Rh(21)−S(21)−N(21)	−51.2(6)
C(32)−Rh(21)−S(21)−N(21)	−91.0(7)
C(35)−Rh(21)−S(21)−N(21)	−26.5(8)
C(34)−Rh(21)−S(21)−N(21)	−77.0(16)
S(24)−Rh(21)−S(21)−N(21)	150.3(5)
S(23)−Rh(21)−S(21)−N(21)	66.6(5)
Rh(22)−Rh(21)−S(21)−N(21)	106.5(5)
C(33)−Rh(21)−S(21)−Rh(22)	136.3(5)
C(31)−Rh(21)−S(21)−Rh(22)	−157.7(4)
C(32)−Rh(21)−S(21)−Rh(22)	162.5(4)
C(35)−Rh(21)−S(21)−Rh(22)	−133.0(6)
C(34)−Rh(21)−S(21)−Rh(22)	176.5(15)
S(24)−Rh(21)−S(21)−Rh(22)	43.76(12)
S(23)−Rh(21)−S(21)−Rh(22)	−39.91(11)
C(33)−Rh(21)−S(24)−S(25)	78.9(4)
C(31)−Rh(21)−S(24)−S(25)	116.0(11)
C(32)−Rh(21)−S(24)−S(25)	112.1(5)
C(35)−Rh(21)−S(24)−S(25)	24.2(8)
C(34)−Rh(21)−S(24)−S(25)	41.2(5)
S(21)−Rh(21)−S(24)−S(25)	−151.2(2)
S(23)−Rh(21)−S(24)−S(25)	−67.88(18)
Rh(22)−Rh(21)−S(24)−S(25)	−107.5(2)
C(33)−Rh(21)−S(24)−Rh(22)	−173.6(4)
C(31)−Rh(21)−S(24)−Rh(22)	−136.5(10)
C(32)−Rh(21)−S(24)−Rh(22)	−140.4(4)
C(35)−Rh(21)−S(24)−Rh(22)	131.8(8)
C(34)−Rh(21)−S(24)−Rh(22)	148.7(5)
S(21)−Rh(21)−S(24)−Rh(22)	−43.71(12)
S(23)−Rh(21)−S(24)−Rh(22)	39.63(11)
C(23)−Rh(22)−S(24)−S(25)	−78.3(4)
C(24)−Rh(22)−S(24)−S(25)	−40.0(5)
C(22)−Rh(22)−S(24)−S(25)	−112.6(4)
C(21)−Rh(22)−S(24)−S(25)	−115.1(10)
C(25)−Rh(22)−S(24)−S(25)	−23.7(8)
S(21)−Rh(22)−S(24)−S(25)	150.5(2)
S(23)−Rh(22)−S(24)−S(25)	67.15(19)
Rh(21)−Rh(22)−S(24)−S(25)	106.8(2)
C(23)−Rh(22)−S(24)−Rh(21)	174.9(4)
C(24)−Rh(22)−S(24)−Rh(21)	−146.8(4)
C(22)−Rh(22)−S(24)−Rh(21)	140.6(4)

Table 6.6 continued

C(21)−Rh(22)−S(24)−Rh(21)	138.1(10)
C(25)−Rh(22)−S(24)−Rh(21)	−130.5(7)
S(21)−Rh(22)−S(24)−Rh(21)	43.73(12)
S(23)−Rh(22)−S(24)−Rh(21)	−39.65(12)
Rh(21)−S(24)−S(25)−O(23)	42.9(5)
Rh(22)−S(24)−S(25)−O(23)	−45.5(5)
Rh(21)−S(24)−S(25)−O(21)	163.1(4)
Rh(22)−S(24)−S(25)−O(21)	74.7(5)
Rh(21)−S(24)−S(25)−O(22)	−79.1(5)
Rh(22)−S(24)−S(25)−O(22)	−167.5(5)
C(23)−Rh(22)−C(21)−C(25)	81.9(8)
C(24)−Rh(22)−C(21)−C(25)	38.3(8)
C(22)−Rh(22)−C(21)−C(25)	119.5(11)
S(21)−Rh(22)−C(21)−C(25)	−147.2(7)
S(23)−Rh(22)−C(21)−C(25)	−59.5(8)
S(24)−Rh(22)−C(21)−C(25)	123.1(11)
Rh(21)−Rh(22)−C(21)−C(25)	−118.7(8)
C(23)−Rh(22)−C(21)−C(22)	−37.6(7)
C(24)−Rh(22)−C(21)−C(22)	−81.2(8)
C(25)−Rh(22)−C(21)−C(22)	−119.5(11)
S(21)−Rh(22)−C(21)−C(22)	93.3(7)
S(23)−Rh(22)−C(21)−C(22)	−179.0(6)
S(24)−Rh(22)−C(21)−C(22)	3.5(14)
Rh(21)−Rh(22)−C(21)−C(22)	121.8(7)
C(23)−Rh(22)−C(21)−C(26)	−157.8(17)
C(24)−Rh(22)−C(21)−C(26)	158.6(17)
C(22)−Rh(22)−C(21)−C(26)	−120.1(18)
C(25)−Rh(22)−C(21)−C(26)	120.3(18)
S(21)−Rh(22)−C(21)−C(26)	−26.9(15)
S(23)−Rh(22)−C(21)−C(26)	60.8(15)
S(24)−Rh(22)−C(21)−C(26)	−116.6(13)
Rh(21)−Rh(22)−C(21)−C(26)	(2)
C(25)−C(21)−C(22)−C(23)	−1.1(15)
C(26)−C(21)−C(22)−C(23)	−176.5(14)
Rh(22)−C(21)−C(22)−C(23)	60.3(9)
C(25)−C(21)−C(22)−C(27)	177.0(13)
C(26)−C(21)−C(22)−C(27)	(2)
Rh(22)−C(21)−C(22)−C(27)	−121.6(14)
C(25)−C(21)−C(22)−Rh(22)	−61.4(10)
C(26)−C(21)−C(22)−Rh(22)	123.2(14)
C(23)−Rh(22)−C(22)−C(21)	118.0(11)
C(24)−Rh(22)−C(22)−C(21)	79.9(8)
C(25)−Rh(22)−C(22)−C(21)	36.3(7)
S(21)−Rh(22)−C(22)−C(21)	−95.0(7)

Table 6.6 continued

S(23)−Rh(22)−C(22)−C(21)	2.3(14)
S(24)−Rh(22)−C(22)−C(21)	−178.5(6)
Rh(21)−Rh(22)−C(22)−C(21)	−119.4(8)
C(24)−Rh(22)−C(22)−C(23)	−38.1(8)
C(21)−Rh(22)−C(22)−C(23)	−118.0(11)
C(25)−Rh(22)−C(22)−C(23)	−81.7(8)
S(21)−Rh(22)−C(22)−C(23)	147.0(7)
S(23)−Rh(22)−C(22)−C(23)	−115.7(10)
S(24)−Rh(22)−C(22)−C(23)	63.5(9)
Rh(21)−Rh(22)−C(22)−C(23)	122.7(8)
C(23)−Rh(22)−C(22)−C(27)	−120.6(15)
C(24)−Rh(22)−C(22)−C(27)	−158.6(13)
C(21)−Rh(22)−C(22)−C(27)	121.4(14)
C(25)−Rh(22)−C(22)−C(27)	157.7(13)
S(21)−Rh(22)−C(22)−C(27)	26.4(12)
S(23)−Rh(22)−C(22)−C(27)	123.7(11)
S(24)−Rh(22)−C(22)−C(27)	−57.0(12)
Rh(21)−Rh(22)−C(22)−C(27)	2.1(15)
C(21)−C(22)−C(23)−C(24)	0.2(15)
C(27)−C(22)−C(23)−C(24)	−177.9(14)
Rh(22)−C(22)−C(23)−C(24)	61.5(10)
C(21)−C(22)−C(23)−C(28)	175.4(14)
C(27)−C(22)−C(23)−C(28)	(2)
Rh(22)−C(22)−C(23)−C(28)	−123.3(15)
C(21)−C(22)−C(23)−Rh(22)	−61.3(9)
C(27)−C(22)−C(23)−Rh(22)	120.5(14)
C(24)−Rh(22)−C(23)−C(22)	117.8(11)
C(21)−Rh(22)−C(23)−C(22)	37.2(8)
C(25)−Rh(22)−C(23)−C(22)	79.2(8)
S(21)−Rh(22)−C(23)−C(22)	−45.8(9)
S(23)−Rh(22)−C(23)−C(22)	142.8(7)
S(24)−Rh(22)−C(23)−C(22)	−128.3(7)
Rh(21)−Rh(22)−C(23)−C(22)	−121.2(7)
C(22)−Rh(22)−C(23)−C(24)	−117.8(11)
C(21)−Rh(22)−C(23)−C(24)	−80.5(8)
C(25)−Rh(22)−C(23)−C(24)	−38.5(7)
S(21)−Rh(22)−C(23)−C(24)	−163.6(6)
S(23)−Rh(22)−C(23)−C(24)	25.0(10)
S(24)−Rh(22)−C(23)−C(24)	114.0(7)
Rh(21)−Rh(22)−C(23)−C(24)	121.0(8)
C(24)−Rh(22)−C(23)−C(28)	−117.2(15)
C(22)−Rh(22)−C(23)−C(28)	125.1(17)
C(21)−Rh(22)−C(23)−C(28)	162.3(15)
C(25)−Rh(22)−C(23)−C(28)	−155.7(14)

Table 6.6 continued

S(21)−Rh(22)−C(23)−C(28)	79.3(13)
S(23)−Rh(22)−C(23)−C(28)	−92.1(14)
S(24)−Rh(22)−C(23)−C(28)	−3.2(13)
Rh(21)−Rh(22)−C(23)−C(28)	3.8(17)
C(22)−C(23)−C(24)−C(29)	174.1(14)
C(28)−C(23)−C(24)−C(29)	(2)
Rh(22)−C(23)−C(24)−C(29)	−123.5(15)
C(22)−C(23)−C(24)−C(25)	0.8(16)
C(28)−C(23)−C(24)−C(25)	−174.7(13)
Rh(22)−C(23)−C(24)−C(25)	63.2(10)
C(22)−C(23)−C(24)−Rh(22)	−62.4(9)
C(28)−C(23)−C(24)−Rh(22)	122.1(13)
C(22)−Rh(22)−C(24)−C(23)	37.4(7)
C(21)−Rh(22)−C(24)−C(23)	79.7(8)
C(25)−Rh(22)−C(24)−C(23)	116.7(11)
S(21)−Rh(22)−C(24)−C(23)	57.6(18)
S(23)−Rh(22)−C(24)−C(23)	−165.5(6)
S(24)−Rh(22)−C(24)−C(23)	−76.5(7)
Rh(21)−Rh(22)−C(24)−C(23)	−123.5(7)
C(23)−Rh(22)−C(24)−C(29)	121.6(16)
C(22)−Rh(22)−C(24)−C(29)	159.0(15)
C(21)−Rh(22)−C(24)−C(29)	−158.7(15)
C(25)−Rh(22)−C(24)−C(29)	−121.7(17)
S(21)−Rh(22)−C(24)−C(29)	179.2(11)
S(23)−Rh(22)−C(24)−C(29)	−43.9(14)
S(24)−Rh(22)−C(24)−C(29)	45.1(14)
Rh(21)−Rh(22)−C(24)−C(29)	−1.9(18)
C(23)−Rh(22)−C(24)−C(25)	−116.7(11)
C(22)−Rh(22)−C(24)−C(25)	−79.2(9)
C(21)−Rh(22)−C(24)−C(25)	−36.9(8)
S(21)−Rh(22)−C(24)−C(25)	(2)
S(23)−Rh(22)−C(24)−C(25)	77.9(8)
S(24)−Rh(22)−C(24)−C(25)	166.8(7)
Rh(21)−Rh(22)−C(24)−C(25)	119.8(8)
C(22)−C(21)−C(25)−C(30)	179.8(14)
C(26)−C(21)−C(25)−C(30)	(2)
Rh(22)−C(21)−C(25)−C(30)	119.0(15)
C(22)−C(21)−C(25)−C(24)	1.6(16)
C(26)−C(21)−C(25)−C(24)	177.0(14)
Rh(22)−C(21)−C(25)−C(24)	−59.2(10)
C(22)−C(21)−C(25)−Rh(22)	60.8(10)
C(26)−C(21)−C(25)−Rh(22)	−123.8(14)
C(23)−C(24)−C(25)−C(30)	−179.6(14)
C(29)−C(24)−C(25)−C(30)	(2)

Table 6.6 continued

Rh(22)−C(24)−C(25)−C(30)	−117.7(15)
C(23)−C(24)−C(25)−C(21)	−1.4(16)
C(29)−C(24)−C(25)−C(21)	−174.9(14)
Rh(22)−C(24)−C(25)−C(21)	60.5(9)
C(23)−C(24)−C(25)−Rh(22)	−61.9(10)
C(29)−C(24)−C(25)−Rh(22)	124.6(16)
C(23)−Rh(22)−C(25)−C(30)	158.6(13)
C(24)−Rh(22)−C(25)−C(30)	120.2(15)
C(22)−Rh(22)−C(25)−C(30)	−158.6(13)
C(21)−Rh(22)−C(25)−C(30)	−122.0(15)
S(21)−Rh(22)−C(25)−C(30)	−76.5(13)
S(23)−Rh(22)−C(25)−C(30)	9.1(12)
S(24)−Rh(22)−C(25)−C(30)	95.9(13)
Rh(21)−Rh(22)−C(25)−C(30)	−2.0(15)
C(23)−Rh(22)−C(25)−C(21)	−79.3(8)
C(24)−Rh(22)−C(25)−C(21)	−117.8(12)
C(22)−Rh(22)−C(25)−C(21)	−36.6(7)
S(21)−Rh(22)−C(25)−C(21)	45.5(9)
S(23)−Rh(22)−C(25)−C(21)	131.1(7)
S(24)−Rh(22)−C(25)−C(21)	−142.1(7)
Rh(21)−Rh(22)−C(25)−C(21)	120.0(8)
C(23)−Rh(22)−C(25)−C(24)	38.4(8)
C(22)−Rh(22)−C(25)−C(24)	81.2(9)
C(21)−Rh(22)−C(25)−C(24)	117.8(12)
S(21)−Rh(22)−C(25)−C(24)	163.3(7)
S(23)−Rh(22)−C(25)−C(24)	−111.1(8)
S(24)−Rh(22)−C(25)−C(24)	−24.3(13)
Rh(21)−Rh(22)−C(25)−C(24)	−122.2(8)
C(33)−Rh(21)−C(31)−C(35)	−79.9(9)
C(32)−Rh(21)−C(31)−C(35)	−115.9(12)
C(34)−Rh(21)−C(31)−C(35)	−37.3(8)
S(21)−Rh(21)−C(31)−C(35)	150.2(7)
S(24)−Rh(21)−C(31)−C(35)	−121.3(11)
S(23)−Rh(21)−C(31)−C(35)	63.1(8)
Rh(22)−Rh(21)−C(31)−C(35)	121.0(8)
C(33)−Rh(21)−C(31)−C(32)	36.0(8)
C(35)−Rh(21)−C(31)−C(32)	115.9(12)
C(34)−Rh(21)−C(31)−C(32)	78.6(9)
S(21)−Rh(21)−C(31)−C(32)	−93.8(8)
S(24)−Rh(21)−C(31)−C(32)	−5.3(16)
S(23)−Rh(21)−C(31)−C(32)	179.0(7)
Rh(22)−Rh(21)−C(31)−C(32)	−123.1(8)
C(33)−Rh(21)−C(31)−C(36)	156.9(15)
C(32)−Rh(21)−C(31)−C(36)	120.9(17)

Table 6.6 continued

C(35)−Rh(21)−C(31)−C(36)	−123.2(17)
C(34)−Rh(21)−C(31)−C(36)	−160.5(15)
S(21)−Rh(21)−C(31)−C(36)	27.1(14)
S(24)−Rh(21)−C(31)−C(36)	115.6(14)
S(23)−Rh(21)−C(31)−C(36)	−60.1(14)
Rh(22)−Rh(21)−C(31)−C(36)	−2.2(18)
C(35)−C(31)−C(32)−C(33)	2.3(17)
C(36)−C(31)−C(32)−C(33)	175.7(14)
Rh(21)−C(31)−C(32)−C(33)	−60.7(11)
C(35)−C(31)−C(32)−C(37)	−177.3(13)
C(36)−C(31)−C(32)−C(37)	(2)
Rh(21)−C(31)−C(32)−C(37)	119.6(14)
C(35)−C(31)−C(32)−Rh(21)	63.1(10)
C(36)−C(31)−C(32)−Rh(21)	−123.5(15)
C(31)−Rh(21)−C(32)−C(33)	119.0(13)
C(35)−Rh(21)−C(32)−C(33)	80.9(10)
C(34)−Rh(21)−C(32)−C(33)	37.7(9)
S(21)−Rh(21)−C(32)−C(33)	−146.6(9)
S(24)−Rh(21)−C(32)−C(33)	−63.2(10)
S(23)−Rh(21)−C(32)−C(33)	116.7(11)
Rh(22)−Rh(21)−C(32)−C(33)	−122.6(8)
C(33)−Rh(21)−C(32)−C(31)	−119.0(13)
C(35)−Rh(21)−C(32)−C(31)	−38.1(8)
C(34)−Rh(21)−C(32)−C(31)	−81.4(9)
S(21)−Rh(21)−C(32)−C(31)	94.4(8)
S(24)−Rh(21)−C(32)−C(31)	177.8(7)
S(23)−Rh(21)−C(32)−C(31)	−2.3(16)
Rh(22)−Rh(21)−C(32)−C(31)	118.4(9)
C(33)−Rh(21)−C(32)−C(37)	123.5(17)
C(31)−Rh(21)−C(32)−C(37)	−117.5(15)
C(35)−Rh(21)−C(32)−C(37)	−155.6(14)
C(34)−Rh(21)−C(32)−C(37)	161.2(14)
S(21)−Rh(21)−C(32)−C(37)	−23.0(12)
S(24)−Rh(21)−C(32)−C(37)	60.3(13)
S(23)−Rh(21)−C(32)−C(37)	−119.8(13)
Rh(22)−Rh(21)−C(32)−C(37)	1.0(17)
C(31)−C(32)−C(33)−C(34)	−2.4(18)
C(37)−C(32)−C(33)−C(34)	177.2(14)
Rh(21)−C(32)−C(33)−C(34)	−62.8(11)
C(31)−C(32)−C(33)−C(38)	−179.8(14)
C(37)−C(32)−C(33)−C(38)	(3)
Rh(21)−C(32)−C(33)−C(38)	119.8(16)
C(31)−C(32)−C(33)−Rh(21)	60.3(11)
C(37)−C(32)−C(33)−Rh(21)	−120.0(16)

Table 6.6 continued

C(31)−Rh(21)−C(33)−C(32)	−37.7(9)
C(35)−Rh(21)−C(33)−C(32)	−80.0(10)
C(34)−Rh(21)−C(33)−C(32)	−118.1(13)
S(21)−Rh(21)−C(33)−C(32)	45.5(11)
S(24)−Rh(21)−C(33)−C(32)	128.5(9)
S(23)−Rh(21)−C(33)−C(32)	−141.4(8)
Rh(22)−Rh(21)−C(33)−C(32)	119.6(9)
C(31)−Rh(21)−C(33)−C(34)	80.4(9)
C(32)−Rh(21)−C(33)−C(34)	118.1(13)
C(35)−Rh(21)−C(33)−C(34)	38.0(9)
S(21)−Rh(21)−C(33)−C(34)	163.5(7)
S(24)−Rh(21)−C(33)−C(34)	−113.5(8)
S(23)−Rh(21)−C(33)−C(34)	−23.4(12)
Rh(22)−Rh(21)−C(33)−C(34)	−122.4(9)
C(31)−Rh(21)−C(33)−C(38)	−160.9(14)
C(32)−Rh(21)−C(33)−C(38)	−123.2(17)
C(35)−Rh(21)−C(33)−C(38)	156.7(14)
C(34)−Rh(21)−C(33)−C(38)	118.7(16)
S(21)−Rh(21)−C(33)−C(38)	−77.7(13)
S(24)−Rh(21)−C(33)−C(38)	5.2(13)
S(23)−Rh(21)−C(33)−C(38)	95.3(14)
Rh(22)−Rh(21)−C(33)−C(38)	−3.7(17)
C(32)−C(33)−C(34)−C(35)	1.6(17)
C(38)−C(33)−C(34)−C(35)	179.1(14)
Rh(21)−C(33)−C(34)−C(35)	−61.0(10)
C(32)−C(33)−C(34)−C(39)	−173.7(15)
C(38)−C(33)−C(34)−C(39)	(2)
Rh(21)−C(33)−C(34)−C(39)	123.7(17)
C(32)−C(33)−C(34)−Rh(21)	62.6(11)
C(38)−C(33)−C(34)−Rh(21)	−119.9(14)
C(31)−Rh(21)−C(34)−C(33)	−80.4(9)
C(32)−Rh(21)−C(34)−C(33)	−36.7(8)
C(35)−Rh(21)−C(34)−C(33)	−117.3(13)
S(21)−Rh(21)−C(34)−C(33)	−52.1(19)
S(24)−Rh(21)−C(34)−C(33)	77.0(8)
S(23)−Rh(21)−C(34)−C(33)	166.7(7)
Rh(22)−Rh(21)−C(34)−C(33)	123.0(8)
C(33)−Rh(21)−C(34)−C(35)	117.3(13)
C(31)−Rh(21)−C(34)−C(35)	36.8(9)
C(32)−Rh(21)−C(34)−C(35)	80.5(10)
S(21)−Rh(21)−C(34)−C(35)	65.1(19)
S(24)−Rh(21)−C(34)−C(35)	−165.7(8)
S(23)−Rh(21)−C(34)−C(35)	−76.0(9)
Rh(22)−Rh(21)−C(34)−C(35)	−119.8(9)

Table 6.6 continued

C(33)−Rh(21)−C(34)−C(39)	−124.7(17)
C(31)−Rh(21)−C(34)−C(39)	154.8(16)
C(32)−Rh(21)−C(34)−C(39)	−161.4(15)
C(35)−Rh(21)−C(34)−C(39)	118.0(18)
S(21)−Rh(21)−C(34)−C(39)	−176.8(10)
S(24)−Rh(21)−C(34)−C(39)	−47.7(14)
S(23)−Rh(21)−C(34)−C(39)	42.0(14)
Rh(22)−Rh(21)−C(34)−C(39)	−1.7(19)
C(32)−C(31)−C(35)−C(34)	−1.3(16)
C(36)−C(31)−C(35)−C(34)	−174.6(14)
Rh(21)−C(31)−C(35)−C(34)	61.1(10)
C(32)−C(31)−C(35)−C(40)	176.3(14)
C(36)−C(31)−C(35)−C(40)	(2)
Rh(21)−C(31)−C(35)−C(40)	−121.3(15)
C(32)−C(31)−C(35)−Rh(21)	−62.4(10)
C(36)−C(31)−C(35)−Rh(21)	124.3(16)
C(33)−C(34)−C(35)−C(31)	−0.1(17)
C(39)−C(34)−C(35)−C(31)	175.5(14)
Rh(21)−C(34)−C(35)−C(31)	−60.7(10)
C(33)−C(34)−C(35)−C(40)	−177.7(14)
C(39)−C(34)−C(35)−C(40)	(2)
Rh(21)−C(34)−C(35)−C(40)	121.7(15)
C(33)−C(34)−C(35)−Rh(21)	60.6(10)
C(39)−C(34)−C(35)−Rh(21)	−123.8(15)
C(33)−Rh(21)−C(35)−C(31)	80.9(9)
C(32)−Rh(21)−C(35)−C(31)	39.2(8)
C(34)−Rh(21)−C(35)−C(31)	118.6(13)
S(21)−Rh(21)−C(35)−C(31)	−41.7(10)
S(24)−Rh(21)−C(35)−C(31)	144.4(8)
S(23)−Rh(21)−C(35)−C(31)	−127.9(8)
Rh(22)−Rh(21)−C(35)−C(31)	−117.8(9)
C(33)−Rh(21)−C(35)−C(34)	−37.7(9)
C(31)−Rh(21)−C(35)−C(34)	−118.6(13)
C(32)−Rh(21)−C(35)−C(34)	−79.4(10)
S(21)−Rh(21)−C(35)−C(34)	−160.3(7)
S(24)−Rh(21)−C(35)−C(34)	25.8(14)
S(23)−Rh(21)−C(35)−C(34)	113.5(9)
Rh(22)−Rh(21)−C(35)−C(34)	123.6(8)
C(33)−Rh(21)−C(35)−C(40)	−159.2(16)
C(31)−Rh(21)−C(35)−C(40)	119.9(17)
C(32)−Rh(21)−C(35)−C(40)	159.1(15)
C(34)−Rh(21)−C(35)−C(40)	−121.5(18)
S(21)−Rh(21)−C(35)−C(40)	78.2(15)
S(24)−Rh(21)−C(35)−C(40)	−95.7(13)

Table 6.6 continued

S(23)−Rh(21)−C(35)−C(40)	−8.0(14)
Rh(22)−Rh(21)−C(35)−C(40)	2.1(19)
Cl(2)−C(41)−Cl(1)−Cl(4)≡1	(3)
Cl(5)−C(42)−Cl(3)−Cl(6)	(4)
Cl(4)−C(42)−Cl(3)−Cl(6)	(4)
Cl(6)−C(42)−Cl(4)−Cl(5)	(3)
Cl(3)−C(42)−Cl(4)−Cl(5)	(4)
Cl(5)−C(42)−Cl(4)−Cl(1)≡2	(12)
Cl(6)−C(42)−Cl(4)−Cl(1)≡2	(11)
Cl(3)−C(42)−Cl(4)−Cl(1)≡2	(10)
Cl(1)≡2−Cl(4)−Cl(5)−C(42)	(3)
C(42)−Cl(4)−Cl(5)−Cl(6)	43.7(17)
Cl(1)≡2−Cl(4)−Cl(5)−Cl(6)	(2)
Cl(6)−C(42)−Cl(5)−Cl(4)	(3)
Cl(3)−C(42)−Cl(5)−Cl(4)	(4)
Cl(4)−C(42)−Cl(5)−Cl(6)	(3)
Cl(3)−C(42)−Cl(5)−Cl(6)	26.2(19)
C(42)−Cl(3)−Cl(6)−Cl(5)	(2)
Cl(5)−C(42)−Cl(6)−Cl(3)	(4)
Cl(4)−C(42)−Cl(6)−Cl(3)	(3)
Cl(4)−C(42)−Cl(6)−Cl(5)	(2)
Cl(3)−C(42)−Cl(6)−Cl(5)	(4)
Cl(4)−Cl(5)−Cl(6)−Cl(3)	(3)
C(42)−Cl(5)−Cl(6)−Cl(3)	(4)
Cl(4)−Cl(5)−Cl(6)−C(42)	(4)

Symmetry transformations used to generate equivalent atoms: #1 $-x+1$, $y+1/2$, $-z+3/2$; #2 $-x+1$, $y-1/2$, $-z+3/2$.

7 Full X-ray data of Cp*Ir[S_2N_2($IrCl_2$Cp*)]·^{n}Bu_2SnCl_2

Table 7.1 Crystal data and structure refinement for Cp*Ir[S_2N_2($IrCl_2$Cp*)] · ^{n}Bu_2SnCl_2 (**54**)

Identification code	vmdw3	
Empirical formula	C31.50 H52 Cl4 Ir2 N2 S2 Sn	
Formula weight	1167.76	
Temperature	93(2) K	
Wavelength	0.710 73 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 10.1044(8) Å	α = 78.220(8)°
	b = 12.1259(13) Å	β = 80.344(8)°
	c = 16.8451(18) Å	γ = 77.688(9)°
Volume	1957.3(3) Å^3	
Z	2	
Density (calculated)	1.981 Mg/m^3	
Absorption coefficient	7.819 mm^{-1}	
F(000)	1118	
Crystal size	0.1000 × 0.0300 × 0.0300 mm^3	
Theta range for data collection	2.28 to 25.35°	
Index ranges	$-10 \leq h \leq 12, -14 \leq k \leq 14, -17 \leq l \leq 20$	
Reflections collected	12710	
Independent reflections	6883 [R(int) = 0.0184]	
Completeness to theta = 25.00°	96.1 %	
Absorption correction	Multiscan	
Max. and min. transmission	1.0000 and 0.7567	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6883 / 0 / 389	
Goodness-of-fit on F^2	1.054	
Final R indices [I>2sigma(I)]	R1 = 0.0220, wR2 = 0.0445	
R indices (all data)	R1 = 0.0256, wR2 = 0.0459	
Largest diff. peak and hole	1.145 and −1.017 e·Å^{-3}	

Table 7.2 Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters (Å$^2\times 10^3$) for Cp*Ir[S_2N_2($IrCl_2$Cp*)] · ^{n}Bu_2SnCl_2 (**54**). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ir(1)	998(1)	7527(1)	3688(1)	9(1)
N(1)	2354(3)	7826(3)	2724(2)	17(1)
S(1)	2727(1)	7000(1)	2096(1)	15(1)
N(2)	1871(3)	5973(3)	2353(2)	11(1)
S(2)	769(1)	6027(1)	3227(1)	13(1)
C(1)	-732(4)	8676(3)	4206(2)	14(1)
C(2)	486(4)	9176(3)	4139(2)	16(1)
C(3)	1414(4)	8393(3)	4621(2)	14(1)
C(4)	778(4)	7409(3)	5014(2)	12(1)
C(5)	-550(4)	7603(3)	4765(2)	12(1)
C(6)	-1991(4)	9205(4)	3813(3)	20(1)
C(7)	722(4)	10310(3)	3634(3)	22(1)
C(8)	2799(4)	8520(4)	4759(3)	24(1)
C(9)	1399(4)	6423(4)	5605(2)	19(1)
C(10)	-1591(4)	6839(4)	5048(3)	17(1)
Ir(2)	1935(1)	4811(1)	1572(1)	8(1)
Cl(1)	4391(1)	4597(1)	1449(1)	13(1)
Cl(2)	1956(1)	3336(1)	2783(1)	13(1)
C(11)	411(4)	5920(3)	880(2)	10(1)
C(12)	-57(4)	4872(3)	1277(2)	10(1)
C(13)	882(4)	3936(3)	953(2)	11(1)
C(14)	1933(4)	4392(3)	386(2)	11(1)
C(15)	1659(4)	5637(3)	346(2)	9(1)
C(16)	-262(4)	7094(3)	1028(2)	16(1)
C(17)	-1307(4)	4773(4)	1886(2)	16(1)
C(18)	763(4)	2695(3)	1189(2)	16(1)
C(19)	3117(4)	3719(3)	-81(2)	15(1)
C(20)	2498(4)	6451(3)	-184(2)	14(1)
Sn(1)	-5081(1)	12594(1)	2841(1)	12(1)
Cl(3)	-2564(1)	12173(1)	2677(1)	19(1)
Cl(4)	-5511(1)	11088(1)	3979(1)	19(1)
C(21)	-5362(4)	13955(3)	3521(2)	16(1)
C(22)	-4453(4)	14851(3)	3233(2)	16(1)
C(23)	-4750(4)	15763(3)	3770(3)	18(1)
C(24)	-3919(5)	16712(4)	3439(3)	28(1)
C(25)	-5202(4)	11818(4)	1826(3)	19(1)
C(26)	-4858(4)	10520(4)	1955(3)	20(1)
C(27)	-4988(5)	10085(4)	1193(3)	26(1)
C(28)	-4545(5)	8797(4)	1256(3)	34(1)
C(31)	1240(10)	9750(7)	211(8)	123(6)
C(32)	136(11)	9992(6)	798(8)	117(5)

Table 7.2 continued

C(33)	-1180(12)	10267(7)	550(10)	140(7)
C(34)	137(12)	9958(9)	1471(8)	36(3)

Table 7.3 Bond lengths [Å] and angles [°] for Cp*Ir[S_2N_2(IrCl_2Cp*)] · ^{n}Bu_2SnCl_2

Ir(1)−N(1)	1.969(3)
Ir(1)−C(1)	2.169(4)
Ir(1)−C(4)	2.184(4)
Ir(1)−S(2)	2.1864(10)
Ir(1)−C(5)	2.190(3)
Ir(1)−C(3)	2.199(4)
Ir(1)−C(2)	2.212(4)
N(1)−S(1)	1.550(3)
S(1)−N(2)	1.612(3)
N(2)−S(2)	1.694(3)
N(2)−Ir(2)	2.100(3)
C(1)−C(5)	1.438(5)
C(1)−C(2)	1.462(5)
C(1)−C(6)	1.494(5)
C(2)−C(3)	1.415(6)
C(2)−C(7)	1.505(5)
C(3)−C(4)	1.463(5)
C(3)−C(8)	1.501(5)
C(4)−C(5)	1.430(5)
C(4)−C(9)	1.489(6)
C(5)−C(10)	1.503(5)
C(6)−H(6A)	0.98
C(6)−H(6B)	0.98
C(6)−H(6C)	0.98
C(7)−H(7A)	0.98
C(7)−H(7B)	0.98
C(7)−H(7C)	0.98
C(8)−H(8A)	0.98
C(8)−H(8B)	0.98
C(8)−H(8C)	0.98
C(9)−H(9A)	0.98
C(9)−H(9B)	0.98
C(9)−H(9C)	0.98
C(10)−H(10A)	0.98
C(10)−H(10B)	0.98
C(10)−H(10C)	0.98
Ir(2)−C(12)	2.135(3)
Ir(2)−C(15)	2.139(4)
Ir(2)−C(11)	2.149(4)
Ir(2)−C(13)	2.157(4)
Ir(2)−C(14)	2.159(4)
Ir(2)−Cl(1)	2.4174(9)
Ir(2)−Cl(2)	2.4222(10)
C(11)−C(15)	1.442(5)

Table 7.3 continued

C(11)−C(12)	1.445(5)
C(11)−C(16)	1.492(5)
C(12)−C(13)	1.452(5)
C(12)−C(17)	1.498(5)
C(13)−C(14)	1.428(5)
C(13)−C(18)	1.501(5)
C(14)−C(15)	1.465(5)
C(14)−C(19)	1.499(5)
C(15)−C(20)	1.494(5)
C(16)−H(16A)	0.98
C(16)−H(16B)	0.98
C(16)−H(16C)	0.98
C(17)−H(17A)	0.98
C(17)−H(17B)	0.98
C(17)−H(17C)	0.98
C(18)−H(18A)	0.98
C(18)−H(18B)	0.98
C(18)−H(18C)	0.98
C(19)−H(19A)	0.98
C(19)−H(19B)	0.98
C(19)−H(19C)	0.98
C(20)−H(20A)	0.98
C(20)−H(20B)	0.98
C(20)−H(20C)	0.98
Sn(1)−C(21)	2.140(4)
Sn(1)−C(25)	2.145(4)
Sn(1)−Cl(4)	2.4133(10)
Sn(1)−Cl(3)	2.4652(10)
C(21)−C(22)	1.524(5)
C(21)−H(21A)	0.99
C(21)−H(21B)	0.99
C(22)−C(23)	1.518(5)
C(22)−H(22A)	0.99
C(22)−H(22B)	0.99
C(23)−C(24)	1.528(5)
C(23)−H(23A)	0.99
C(23)−H(23B)	0.99
C(24)−H(24A)	0.98
C(24)−H(24B)	0.98
C(24)−H(24C)	0.98
C(25)−C(26)	1.516(6)
C(25)−H(25A)	0.99
C(25)−H(25B)	0.99
C(26)−C(27)	1.518(6)

Table 7.3 continued

C(26)−H(26A)	0.99
C(26)−H(26B)	0.99
C(27)−C(28)	1.517(6)
C(27)−H(27A)	0.99
C(27)−H(27B)	0.99
C(28)−H(28A)	0.98
C(28)−H(28B)	0.98
C(28)−H(28C)	0.98
C(31)−C(33)#1	1.30(2)
C(31)−C(32)	1.385(10)
C(31)−H(31A)	0.95
C(32)−C(34)	1.127(15)
C(32)−C(33)	1.412(19)
C(33)−C(31)#1	1.30(2)
C(33)−H(33A)	0.95
C(34)−H(34A)	0.98
C(34)−H(34B)	0.98
C(34)−H(34C)	0.98
N(1)−Ir(1)−C(1)	130.19(14)
N(1)−Ir(1)−C(4)	139.24(13)
C(1)−Ir(1)−C(4)	64.41(15)
N(1)−Ir(1)−S(2)	87.78(9)
C(1)−Ir(1)−S(2)	122.55(10)
C(4)−Ir(1)−S(2)	117.35(10)
N(1)−Ir(1)−C(5)	167.13(14)
C(1)−Ir(1)−C(5)	38.53(14)
C(4)−Ir(1)−C(5)	38.17(14)
S(2)−Ir(1)−C(5)	104.13(10)
N(1)−Ir(1)−C(3)	106.66(13)
C(1)−Ir(1)−C(3)	64.29(14)
C(4)−Ir(1)−C(3)	38.98(14)
S(2)−Ir(1)−C(3)	153.71(11)
C(5)−Ir(1)−C(3)	64.41(14)
N(1)−Ir(1)−C(2)	102.77(14)
C(1)−Ir(1)−C(2)	38.99(14)
C(4)−Ir(1)−C(2)	64.09(15)
S(2)−Ir(1)−C(2)	160.82(11)
C(5)−Ir(1)−C(2)	64.43(14)
C(3)−Ir(1)−C(2)	37.42(15)
S(1)−N(1)−Ir(1)	119.81(18)
N(1)−S(1)−N(2)	111.31(16)
S(1)−N(2)−S(2)	114.68(19)
S(1)−N(2)−Ir(2)	121.66(17)

Table 7.3 continued

S(2)−N(2)−Ir(2)	123.12(16)
N(2)−S(2)−Ir(1)	106.41(11)
C(5)−C(1)−C(2)	108.0(3)
C(5)−C(1)−C(6)	125.1(3)
C(2)−C(1)−C(6)	126.8(4)
C(5)−C(1)−Ir(1)	71.5(2)
C(2)−C(1)−Ir(1)	72.1(2)
C(6)−C(1)−Ir(1)	125.0(3)
C(3)−C(2)−C(1)	107.7(3)
C(3)−C(2)−C(7)	126.1(4)
C(1)−C(2)−C(7)	126.1(4)
C(3)−C(2)−Ir(1)	70.8(2)
C(1)−C(2)−Ir(1)	68.9(2)
C(7)−C(2)−Ir(1)	124.8(3)
C(2)−C(3)−C(4)	108.3(3)
C(2)−C(3)−C(8)	128.1(4)
C(4)−C(3)−C(8)	123.5(4)
C(2)−C(3)−Ir(1)	71.8(2)
C(4)−C(3)−Ir(1)	70.0(2)
C(8)−C(3)−Ir(1)	125.8(3)
C(5)−C(4)−C(3)	107.9(3)
C(5)−C(4)−C(9)	127.2(3)
C(3)−C(4)−C(9)	124.8(3)
C(5)−C(4)−Ir(1)	71.1(2)
C(3)−C(4)−Ir(1)	71.0(2)
C(9)−C(4)−Ir(1)	126.1(3)
C(4)−C(5)−C(1)	108.0(3)
C(4)−C(5)−C(10)	126.3(4)
C(1)−C(5)−C(10)	125.7(3)
C(4)−C(5)−Ir(1)	70.7(2)
C(1)−C(5)−Ir(1)	69.9(2)
C(10)−C(5)−Ir(1)	125.9(3)
C(1)−C(6)−H(6A)	109.5
C(1)−C(6)−H(6B)	109.5
H(6A)−C(6)−H(6B)	109.5
C(1)−C(6)−H(6C)	109.5
H(6A)−C(6)−H(6C)	109.5
H(6B)−C(6)−H(6C)	109.5
C(2)−C(7)−H(7A)	109.5
C(2)−C(7)−H(7B)	109.5
H(7A)−C(7)−H(7B)	109.5
C(2)−C(7)−H(7C)	109.5
H(7A)−C(7)−H(7C)	109.5
H(7B)−C(7)−H(7C)	109.5

Table 7.3 continued

C(3)−C(8)−H(8A)	109.5
C(3)−C(8)−H(8B)	109.5
H(8A)−C(8)−H(8B)	109.5
C(3)−C(8)−H(8C)	109.5
H(8A)−C(8)−H(8C)	109.5
H(8B)−C(8)−H(8C)	109.5
C(4)−C(9)−H(9A)	109.5
C(4)−C(9)−H(9B)	109.5
H(9A)−C(9)−H(9B)	109.5
C(4)−C(9)−H(9C)	109.5
H(9A)−C(9)−H(9C)	109.5
H(9B)−C(9)−H(9C)	109.5
C(5)−C(10)−H(10A)	109.5
C(5)−C(10)−H(10B)	109.5
H(10A)−C(10)−H(10B)	109.5
C(5)−C(10)−H(10C)	109.5
H(10A)−C(10)−H(10C)	109.5
H(10B)−C(10)−H(10C)	109.5
N(2)−Ir(2)−C(12)	110.71(13)
N(2)−Ir(2)−C(15)	112.89(13)
C(12)−Ir(2)−C(15)	66.59(14)
N(2)−Ir(2)−C(11)	94.05(13)
C(12)−Ir(2)−C(11)	39.43(14)
C(15)−Ir(2)−C(11)	39.30(13)
N(2)−Ir(2)−C(13)	149.74(13)
C(12)−Ir(2)−C(13)	39.53(14)
C(15)−Ir(2)−C(13)	66.02(14)
C(11)−Ir(2)−C(13)	65.62(14)
N(2)−Ir(2)−C(14)	152.59(13)
C(12)−Ir(2)−C(14)	66.03(14)
C(15)−Ir(2)−C(14)	39.85(14)
C(11)−Ir(2)−C(14)	65.80(14)
C(13)−Ir(2)−C(14)	38.63(14)
N(2)−Ir(2)−Cl(1)	85.82(8)
C(12)−Ir(2)−Cl(1)	160.75(10)
C(15)−Ir(2)−Cl(1)	98.44(10)
C(11)−Ir(2)−Cl(1)	133.22(10)
C(13)−Ir(2)−Cl(1)	124.43(10)
C(14)−Ir(2)−Cl(1)	94.74(10)
N(2)−Ir(2)−Cl(2)	86.84(9)
C(12)−Ir(2)−Cl(2)	100.01(10)
C(15)−Ir(2)−Cl(2)	158.79(10)
C(11)−Ir(2)−Cl(2)	136.36(10)
C(13)−Ir(2)−Cl(2)	93.09(10)

Table 7.3 continued

C(14)−Ir(2)−Cl(2)	120.53(10)
Cl(1)−Ir(2)−Cl(2)	90.39(3)
C(15)−C(11)−C(12)	108.7(3)
C(15)−C(11)−C(16)	125.9(3)
C(12)−C(11)−C(16)	125.3(3)
C(15)−C(11)−Ir(2)	70.0(2)
C(12)−C(11)−Ir(2)	69.8(2)
C(16)−C(11)−Ir(2)	124.3(3)
C(11)−C(12)−C(13)	107.3(3)
C(11)−C(12)−C(17)	126.4(3)
C(13)−C(12)−C(17)	126.3(3)
C(11)−C(12)−Ir(2)	70.8(2)
C(13)−C(12)−Ir(2)	71.0(2)
C(17)−C(12)−Ir(2)	125.2(3)
C(14)−C(13)−C(12)	108.7(3)
C(14)−C(13)−C(18)	126.2(3)
C(12)−C(13)−C(18)	125.1(3)
C(14)−C(13)−Ir(2)	70.8(2)
C(12)−C(13)−Ir(2)	69.4(2)
C(18)−C(13)−Ir(2)	125.1(3)
C(13)−C(14)−C(15)	108.0(3)
C(13)−C(14)−C(19)	126.3(3)
C(15)−C(14)−C(19)	125.8(3)
C(13)−C(14)−Ir(2)	70.6(2)
C(15)−C(14)−Ir(2)	69.3(2)
C(19)−C(14)−Ir(2)	125.2(3)
C(11)−C(15)−C(14)	107.2(3)
C(11)−C(15)−C(20)	127.1(3)
C(14)−C(15)−C(20)	125.6(3)
C(11)−C(15)−Ir(2)	70.7(2)
C(14)−C(15)−Ir(2)	70.8(2)
C(20)−C(15)−Ir(2)	125.8(3)
C(11)−C(16)−H(16A)	109.5
C(11)−C(16)−H(16B)	109.5
H(16A)−C(16)−H(16B)	109.5
C(11)−C(16)−H(16C)	109.5
H(16A)−C(16)−H(16C)	109.5
H(16B)−C(16)−H(16C)	109.5
C(12)−C(17)−H(17A)	109.5
C(12)−C(17)−H(17B)	109.5
H(17A)−C(17)−H(17B)	109.5
C(12)−C(17)−H(17C)	109.5
H(17A)−C(17)−H(17C)	109.5
H(17B)−C(17)−H(17C)	109.5

Table 7.3 continued

C(13)−C(18)−H(18A)	109.5
C(13)−C(18)−H(18B)	109.5
H(18A)−C(18)−H(18B)	109.5
C(13)−C(18)−H(18C)	109.5
H(18A)−C(18)−H(18C)	109.5
H(18B)−C(18)−H(18C)	109.5
C(14)−C(19)−H(19A)	109.5
C(14)−C(19)−H(19B)	109.5
H(19A)−C(19)−H(19B)	109.5
C(14)−C(19)−H(19C)	109.5
H(19A)−C(19)−H(19C)	109.5
H(19B)−C(19)−H(19C)	109.5
C(15)−C(20)−H(20A)	109.5
C(15)−C(20)−H(20B)	109.5
H(20A)−C(20)−H(20B)	109.5
C(15)−C(20)−H(20C)	109.5
H(20A)−C(20)−H(20C)	109.5
H(20B)−C(20)−H(20C)	109.5
C(21)−Sn(1)−C(25)	156.25(16)
C(21)−Sn(1)−Cl(4)	97.73(11)
C(25)−Sn(1)−Cl(4)	101.34(12)
C(21)−Sn(1)−Cl(3)	97.22(10)
C(25)−Sn(1)−Cl(3)	93.77(11)
Cl(4)−Sn(1)−Cl(3)	98.74(4)
C(22)−C(21)−Sn(1)	117.9(3)
C(22)−C(21)−H(21A)	107.8
Sn(1)−C(21)−H(21A)	107.8
C(22)−C(21)−H(21B)	107.8
Sn(1)−C(21)−H(21B)	107.8
H(21A)−C(21)−H(21B)	107.2
C(23)−C(22)−C(21)	112.6(3)
C(23)−C(22)−H(22A)	109.1
C(21)−C(22)−H(22A)	109.1
C(23)−C(22)−H(22B)	109.1
C(21)−C(22)−H(22B)	109.1
H(22A)−C(22)−H(22B)	107.8
C(22)−C(23)−C(24)	112.3(3)
C(22)−C(23)−H(23A)	109.1
C(24)−C(23)−H(23A)	109.1
C(22)−C(23)−H(23B)	109.1
C(24)−C(23)−H(23B)	109.1
H(23A)−C(23)−H(23B)	107.9
C(23)−C(24)−H(24A)	109.5
C(23)−C(24)−H(24B)	109.5

Table 7.3 continued

H(24A)−C(24)−H(24B)	109.5
C(23)−C(24)−H(24C)	109.5
H(24A)−C(24)−H(24C)	109.5
H(24B)−C(24)−H(24C)	109.5
C(26)−C(25)−Sn(1)	116.3(3)
C(26)−C(25)−H(25A)	108.2
Sn(1)−C(25)−H(25A)	108.2
C(26)−C(25)−H(25B)	108.2
Sn(1)−C(25)−H(25B)	108.2
H(25A)−C(25)−H(25B)	107.4
C(25)−C(26)−C(27)	110.9(4)
C(25)−C(26)−H(26A)	109.5
C(27)−C(26)−H(26A)	109.5
C(25)−C(26)−H(26B)	109.5
C(27)−C(26)−H(26B)	109.5
H(26A)−C(26)−H(26B)	108.1
C(28)−C(27)−C(26)	113.5(4)
C(28)−C(27)−H(27A)	108.9
C(26)−C(27)−H(27A)	108.9
C(28)−C(27)−H(27B)	108.9
C(26)−C(27)−H(27B)	108.9
H(27A)−C(27)−H(27B)	107.7
C(27)−C(28)−H(28A)	109.5
C(27)−C(28)−H(28B)	109.5
H(28A)−C(28)−H(28B)	109.5
C(27)−C(28)−H(28C)	109.5
H(28A)−C(28)−H(28C)	109.5
H(28B)−C(28)−H(28C)	109.5
C(33)#1−C(31)−C(32)	126.0(14)
C(33)#1−C(31)−H(31A)	117
C(32)−C(31)−H(31A)	117
C(34)−C(32)−C(31)	128.2(16)
C(34)−C(32)−C(33)	114.1(11)
C(31)−C(32)−C(33)	117.6(13)
C(31)#1−C(33)−C(32)	116.4(10)
C(31)#1−C(33)−H(33A)	121.8
C(32)−C(33)−H(33A)	121.8
C(32)−C(34)−H(34A)	109.5
C(32)−C(34)−H(34B)	109.5
H(34A)−C(34)−H(34B)	109.5
C(32)−C(34)−H(34C)	109.5
H(34A)−C(34)−H(34C)	109.5
H(34B)−C(34)−H(34C)	109.5

Symmetry transformations used to generate equivalent atoms: $\#1 - x, -y + 2, -z$

Table 7.4 Anisotropic displacement parameters (Å$^2\times10^3$) for Cp*Ir[S_2N_2(IrCl_2Cp*)] · ^{n}Bu$_2$SnCl_2 (**54**). The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2\ a^{*2}\ U^{11} + \ldots + 2\ h\ k\ a^*\ b^*\ U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ir(1)	11(1)	9(1)	8(1)	-3(1)	-1(1)	-2(1)
N(1)	23(2)	16(2)	14(2)	-6(2)	1(2)	-10(2)
S(1)	19(1)	14(1)	13(1)	-6(1)	5(1)	-8(1)
N(2)	11(2)	12(2)	10(2)	-5(1)	1(1)	-2(1)
S(2)	16(1)	14(1)	12(1)	-7(1)	4(1)	-6(1)
C(1)	16(2)	11(2)	14(2)	-10(2)	0(2)	4(2)
C(2)	25(2)	12(2)	12(2)	-7(2)	0(2)	-4(2)
C(3)	17(2)	14(2)	14(2)	-9(2)	-1(2)	-4(2)
C(4)	18(2)	15(2)	7(2)	-10(2)	0(2)	-3(2)
C(5)	15(2)	11(2)	8(2)	-3(2)	3(2)	-1(2)
C(6)	21(2)	14(2)	23(2)	-4(2)	-6(2)	3(2)
C(7)	32(2)	11(2)	21(2)	-2(2)	0(2)	-7(2)
C(8)	26(2)	25(3)	25(3)	-9(2)	-9(2)	-8(2)
C(9)	23(2)	21(2)	13(2)	-2(2)	-7(2)	-2(2)
C(10)	16(2)	21(2)	17(2)	-6(2)	0(2)	-5(2)
Ir(2)	9(1)	8(1)	6(1)	-2(1)	0(1)	-2(1)
Cl(1)	11(1)	17(1)	10(1)	-3(1)	-1(1)	-2(1)
Cl(2)	16(1)	12(1)	10(1)	1(1)	-2(1)	-4(1)
C(11)	11(2)	12(2)	7(2)	-2(2)	-4(2)	-1(2)
C(12)	10(2)	15(2)	9(2)	-4(2)	-3(2)	-5(2)
C(13)	15(2)	14(2)	8(2)	-3(2)	-7(2)	-4(2)
C(14)	13(2)	16(2)	5(2)	-2(2)	-5(2)	-3(2)
C(15)	15(2)	7(2)	5(2)	-1(2)	-5(2)	0(2)
C(16)	16(2)	13(2)	17(2)	-4(2)	-2(2)	1(2)
C(17)	12(2)	18(2)	16(2)	-5(2)	4(2)	-5(2)
C(18)	19(2)	14(2)	17(2)	-8(2)	-1(2)	-4(2)
C(19)	19(2)	13(2)	11(2)	-6(2)	0(2)	1(2)
C(20)	17(2)	16(2)	10(2)	0(2)	0(2)	-5(2)
Sn(1)	12(1)	10(1)	11(1)	-1(1)	-1(1)	-1(1)
Cl(3)	12(1)	15(1)	28(1)	-1(1)	2(1)	-3(1)
Cl(4)	21(1)	15(1)	17(1)	2(1)	-1(1)	-5(1)
C(21)	16(2)	21(2)	13(2)	-7(2)	-3(2)	-5(2)
C(22)	16(2)	19(2)	13(2)	-1(2)	-6(2)	-6(2)
C(23)	16(2)	19(2)	19(2)	-4(2)	-4(2)	-4(2)
C(24)	37(3)	24(3)	29(3)	-6(2)	-10(2)	-15(2)
C(25)	23(2)	17(2)	19(2)	-10(2)	-6(2)	2(2)
C(26)	25(2)	17(2)	20(2)	-5(2)	-4(2)	-5(2)
C(27)	27(2)	23(3)	27(3)	-11(2)	-3(2)	-2(2)
C(28)	47(3)	23(3)	34(3)	-14(2)	-1(2)	-5(2)
C(31)	74(6)	18(4)	244(15)	-34(7)	95(9)	-20(4)
C(32)	118(8)	16(4)	191(12)	-29(6)	98(9)	-36(5)

Table 7.4 continued

C(33)	86(7)	19(4)	279(18)	-42(7)	122(10)	-27(4)
C(34)	39(6)	7(5)	54(8)	-5(5)	14(6)	-4(4)

Table 7.5 Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters (Å$^2\times 10^3$) for Cp*Ir[S_2N_2($IrCl_2$Cp*)] · ^{n}Bu_2SnCl_2 (**54**)

	x	y	z	U(eq)
H(6A)	-2620	9691	4165	30
H(6B)	-2436	8599	3733	30
H(6C)	-1745	9671	3282	30
H(7A)	419	10910	3970	32
H(7B)	203	10493	3167	32
H(7C)	1698	10264	3435	32
H(8A)	2702	8941	5211	36
H(8B)	3238	8942	4261	36
H(8C)	3361	7759	4897	36
H(9A)	1138	6591	6161	28
H(9B)	2396	6298	5475	28
H(9C)	1072	5733	5568	28
H(10A)	-2156	7050	5546	26
H(10B)	-1122	6039	5163	26
H(10C)	-2172	6929	4619	26
H(16A)	-918	7433	638	24
H(16B)	432	7573	957	24
H(16C)	-741	7047	1587	24
H(17A)	-2090	4825	1599	23
H(17B)	-1488	5397	2202	23
H(17C)	-1161	4035	2257	23
H(18A)	237	2504	814	24
H(18B)	298	2554	1749	24
H(18C)	1678	2218	1158	24
H(19A)	2859	3648	-601	22
H(19B)	3372	2954	241	22
H(19C)	3896	4116	-188	22
H(20A)	2162	6706	-716	22
H(20B)	3455	6064	-261	22
H(20C)	2429	7116	78	22
H(21A)	-6324	14358	3526	19
H(21B)	-5228	13607	4094	19
H(22A)	-3484	14466	3231	19
H(22B)	-4588	15224	2665	19
H(23A)	-4540	15400	4328	21
H(23B)	-5736	16104	3809	21
H(24A)	-4145	17280	3803	42
H(24B)	-4138	17085	2891	42
H(24C)	-2943	16381	3410	42
H(25A)	-6141	12065	1678	23
H(25B)	-4576	12122	1353	23
H(26A)	-5484	10199	2420	24

Table 7.5 continued

H(26B)	-3913	10256	2091	24
H(27A)	-5951	10303	1085	31
H(27B)	-4426	10467	720	31
H(28A)	-4641	8574	745	51
H(28B)	-5119	8411	1710	51
H(28C)	-3588	8575	1356	51
H(31A)	2123	9582	380	147
H(33A)	-1978	10454	920	169
H(34A)	-589	10558	1663	53
H(34B)	1022	10079	1565	53
H(34C)	-23	9206	1772	53

Table 7.6 Torsion angles [°] for Cp*Ir[S_2N_2(IrCl_2Cp*)] · ^{n}Bu$_2$SnCl_2 (**54**)

C(1)−Ir(1)−N(1)−S(1)	−133.3(2)
C(4)−Ir(1)−N(1)−S(1)	130.2(2)
S(2)−Ir(1)−N(1)−S(1)	−1.1(2)
C(5)−Ir(1)−N(1)−S(1)	−159.0(5)
C(3)−Ir(1)−N(1)−S(1)	156.6(2)
C(2)−Ir(1)−N(1)−S(1)	−164.9(2)
Ir(1)−N(1)−S(1)−N(2)	0.6(3)
N(1)−S(1)−N(2)−S(2)	0.5(3)
N(1)−S(1)−N(2)−Ir(2)	172.38(19)
S(1)−N(2)−S(2)−Ir(1)	−1.2(2)
Ir(2)−N(2)−S(2)−Ir(1)	−172.92(14)
N(1)−Ir(1)−S(2)−N(2)	1.16(16)
C(1)−Ir(1)−S(2)−N(2)	139.00(17)
C(4)−Ir(1)−S(2)−N(2)	−145.27(16)
C(5)−Ir(1)−S(2)−N(2)	176.22(16)
C(3)−Ir(1)−S(2)−N(2)	−123.5(2)
C(2)−Ir(1)−S(2)−N(2)	125.3(3)
N(1)−Ir(1)−C(1)−C(5)	−171.1(2)
C(4)−Ir(1)−C(1)−C(5)	−37.1(2)
S(2)−Ir(1)−C(1)−C(5)	70.3(2)
C(3)−Ir(1)−C(1)−C(5)	−80.5(2)
C(2)−Ir(1)−C(1)−C(5)	−116.8(3)
N(1)−Ir(1)−C(1)−C(2)	−54.3(3)
C(4)−Ir(1)−C(1)−C(2)	79.7(2)
S(2)−Ir(1)−C(1)−C(2)	−172.91(18)
C(5)−Ir(1)−C(1)−C(2)	116.8(3)
C(3)−Ir(1)−C(1)−C(2)	36.3(2)
N(1)−Ir(1)−C(1)−C(6)	68.5(4)
C(4)−Ir(1)−C(1)−C(6)	−157.5(4)
S(2)−Ir(1)−C(1)−C(6)	−50.1(4)
C(5)−Ir(1)−C(1)−C(6)	−120.4(4)
C(3)−Ir(1)−C(1)−C(6)	159.1(4)
C(2)−Ir(1)−C(1)−C(6)	122.8(4)
C(5)−C(1)−C(2)−C(3)	2.5(4)
C(6)−C(1)−C(2)−C(3)	178.9(4)
Ir(1)−C(1)−C(2)−C(3)	−60.4(3)
C(5)−C(1)−C(2)−C(7)	−178.6(4)
C(6)−C(1)−C(2)−C(7)	−2.2(6)
Ir(1)−C(1)−C(2)−C(7)	118.4(4)
C(5)−C(1)−C(2)−Ir(1)	62.9(3)
C(6)−C(1)−C(2)−Ir(1)	−120.7(4)
N(1)−Ir(1)−C(2)−C(3)	−100.8(2)
C(1)−Ir(1)−C(2)−C(3)	118.7(3)
C(4)−Ir(1)−C(2)−C(3)	38.1(2)

Table 7.6 continued

S(2)−Ir(1)−C(2)−C(3)	137.2(3)
C(5)−Ir(1)−C(2)−C(3)	80.6(2)
N(1)−Ir(1)−C(2)−C(1)	140.5(2)
C(4)−Ir(1)−C(2)−C(1)	−80.6(2)
S(2)−Ir(1)−C(2)−C(1)	18.5(5)
C(5)−Ir(1)−C(2)−C(1)	−38.1(2)
C(3)−Ir(1)−C(2)−C(1)	−118.7(3)
N(1)−Ir(1)−C(2)−C(7)	20.4(4)
C(1)−Ir(1)−C(2)−C(7)	−120.1(5)
C(4)−Ir(1)−C(2)−C(7)	159.3(4)
S(2)−Ir(1)−C(2)−C(7)	−101.7(4)
C(5)−Ir(1)−C(2)−C(7)	−158.2(4)
C(3)−Ir(1)−C(2)−C(7)	121.2(4)
C(1)−C(2)−C(3)−C(4)	−1.5(4)
C(7)−C(2)−C(3)−C(4)	179.6(4)
Ir(1)−C(2)−C(3)−C(4)	−60.8(3)
C(1)−C(2)−C(3)−C(8)	−179.2(4)
C(7)−C(2)−C(3)−C(8)	2.0(7)
Ir(1)−C(2)−C(3)−C(8)	121.6(4)
C(1)−C(2)−C(3)−Ir(1)	59.2(3)
C(7)−C(2)−C(3)−Ir(1)	−119.6(4)
N(1)−Ir(1)−C(3)−C(2)	89.3(2)
C(1)−Ir(1)−C(3)−C(2)	−37.8(2)
C(4)−Ir(1)−C(3)−C(2)	−118.2(3)
S(2)−Ir(1)−C(3)−C(2)	−149.7(2)
C(5)−Ir(1)−C(3)−C(2)	−80.7(2)
N(1)−Ir(1)−C(3)−C(4)	−152.5(2)
C(1)−Ir(1)−C(3)−C(4)	80.4(2)
S(2)−Ir(1)−C(3)−C(4)	−31.6(4)
C(5)−Ir(1)−C(3)−C(4)	37.4(2)
C(2)−Ir(1)−C(3)−C(4)	118.2(3)
N(1)−Ir(1)−C(3)−C(8)	−35.0(4)
C(1)−Ir(1)−C(3)−C(8)	−162.1(4)
C(4)−Ir(1)−C(3)−C(8)	117.5(5)
S(2)−Ir(1)−C(3)−C(8)	86.0(4)
C(5)−Ir(1)−C(3)−C(8)	155.0(4)
C(2)−Ir(1)−C(3)−C(8)	−124.3(4)
C(2)−C(3)−C(4)−C(5)	0.0(4)
C(8)−C(3)−C(4)−C(5)	177.7(4)
Ir(1)−C(3)−C(4)−C(5)	−61.9(2)
C(2)−C(3)−C(4)−C(9)	−176.8(4)
C(8)−C(3)−C(4)−C(9)	1.0(6)
Ir(1)−C(3)−C(4)−C(9)	121.3(4)
C(2)−C(3)−C(4)−Ir(1)	61.9(3)

Table 7.6 continued

C(8)−C(3)−C(4)−Ir(1)	−120.3(4)
N(1)−Ir(1)−C(4)−C(5)	160.1(2)
C(1)−Ir(1)−C(4)−C(5)	37.4(2)
S(2)−Ir(1)−C(4)−C(5)	−77.7(2)
C(3)−Ir(1)−C(4)−C(5)	117.5(3)
C(2)−Ir(1)−C(4)−C(5)	80.9(2)
N(1)−Ir(1)−C(4)−C(3)	42.7(3)
C(1)−Ir(1)−C(4)−C(3)	−80.0(2)
S(2)−Ir(1)−C(4)−C(3)	164.87(18)
C(5)−Ir(1)−C(4)−C(3)	−117.5(3)
C(2)−Ir(1)−C(4)−C(3)	−36.6(2)
N(1)−Ir(1)−C(4)−C(9)	−77.1(4)
C(1)−Ir(1)−C(4)−C(9)	160.2(4)
S(2)−Ir(1)−C(4)−C(9)	45.1(3)
C(5)−Ir(1)−C(4)−C(9)	122.8(4)
C(3)−Ir(1)−C(4)−C(9)	−119.8(4)
C(2)−Ir(1)−C(4)−C(9)	−156.3(4)
C(3)−C(4)−C(5)−C(1)	1.6(4)
C(9)−C(4)−C(5)−C(1)	178.2(4)
Ir(1)−C(4)−C(5)−C(1)	−60.3(3)
C(3)−C(4)−C(5)−C(10)	−177.2(4)
C(9)−C(4)−C(5)−C(10)	−0.5(6)
Ir(1)−C(4)−C(5)−C(10)	121.0(4)
C(3)−C(4)−C(5)−Ir(1)	61.9(2)
C(9)−C(4)−C(5)−Ir(1)	−121.5(4)
C(2)−C(1)−C(5)−C(4)	−2.5(4)
C(6)−C(1)−C(5)−C(4)	−179.0(3)
Ir(1)−C(1)−C(5)−C(4)	60.8(3)
C(2)−C(1)−C(5)−C(10)	176.2(3)
C(6)−C(1)−C(5)−C(10)	−0.2(6)
Ir(1)−C(1)−C(5)−C(10)	−120.5(4)
C(2)−C(1)−C(5)−Ir(1)	−63.3(3)
C(6)−C(1)−C(5)−Ir(1)	120.3(4)
N(1)−Ir(1)−C(5)−C(4)	−86.2(7)
C(1)−Ir(1)−C(5)−C(4)	−118.4(3)
S(2)−Ir(1)−C(5)−C(4)	116.5(2)
C(3)−Ir(1)−C(5)−C(4)	−38.2(2)
C(2)−Ir(1)−C(5)−C(4)	−79.9(2)
N(1)−Ir(1)−C(5)−C(1)	32.2(7)
C(4)−Ir(1)−C(5)−C(1)	118.4(3)
S(2)−Ir(1)−C(5)−C(1)	−125.1(2)
C(3)−Ir(1)−C(5)−C(1)	80.2(2)
C(2)−Ir(1)−C(5)−C(1)	38.5(2)
N(1)−Ir(1)−C(5)−C(10)	152.4(5)

Table 7.6 continued

C(1)−Ir(1)−C(5)−C(10)	120.2(4)
C(4)−Ir(1)−C(5)−C(10)	−121.4(4)
S(2)−Ir(1)−C(5)−C(10)	−4.9(4)
C(3)−Ir(1)−C(5)−C(10)	−159.7(4)
C(2)−Ir(1)−C(5)−C(10)	158.7(4)
S(1)−N(2)−Ir(2)−C(12)	−120.1(2)
S(2)−N(2)−Ir(2)−C(12)	51.1(2)
S(1)−N(2)−Ir(2)−C(15)	−47.6(2)
S(2)−N(2)−Ir(2)−C(15)	123.6(2)
S(1)−N(2)−Ir(2)−C(11)	−83.3(2)
S(2)−N(2)−Ir(2)−C(11)	87.9(2)
S(1)−N(2)−Ir(2)−C(13)	−128.9(2)
S(2)−N(2)−Ir(2)−C(13)	42.3(4)
S(1)−N(2)−Ir(2)−C(14)	−42.4(4)
S(2)−N(2)−Ir(2)−C(14)	128.8(3)
S(1)−N(2)−Ir(2)−Cl(1)	49.80(19)
S(2)−N(2)−Ir(2)−Cl(1)	−139.0(2)
S(1)−N(2)−Ir(2)−Cl(2)	140.43(19)
S(2)−N(2)−Ir(2)−Cl(2)	−48.37(19)
N(2)−Ir(2)−C(11)−C(15)	122.0(2)
C(12)−Ir(2)−C(11)−C(15)	−119.9(3)
C(13)−Ir(2)−C(11)−C(15)	−81.3(2)
C(14)−Ir(2)−C(11)−C(15)	−38.8(2)
Cl(1)−Ir(2)−C(11)−C(15)	33.9(3)
Cl(2)−Ir(2)−C(11)−C(15)	−148.39(16)
N(2)−Ir(2)−C(11)−C(12)	−118.2(2)
C(15)−Ir(2)−C(11)−C(12)	119.9(3)
C(13)−Ir(2)−C(11)−C(12)	38.6(2)
C(14)−Ir(2)−C(11)−C(12)	81.1(2)
Cl(1)−Ir(2)−C(11)−C(12)	153.76(17)
Cl(2)−Ir(2)−C(11)−C(12)	−28.5(3)
N(2)−Ir(2)−C(11)−C(16)	1.5(3)
C(12)−Ir(2)−C(11)−C(16)	119.6(4)
C(15)−Ir(2)−C(11)−C(16)	−120.5(4)
C(13)−Ir(2)−C(11)−C(16)	158.2(3)
C(14)−Ir(2)−C(11)−C(16)	−159.2(3)
Cl(1)−Ir(2)−C(11)−C(16)	−86.6(3)
Cl(2)−Ir(2)−C(11)−C(16)	91.1(3)
C(15)−C(11)−C(12)−C(13)	−2.7(4)
C(16)−C(11)−C(12)−C(13)	179.6(3)
Ir(2)−C(11)−C(12)−C(13)	−62.1(2)
C(15)−C(11)−C(12)−C(17)	179.4(3)
C(16)−C(11)−C(12)−C(17)	1.7(6)
Ir(2)−C(11)−C(12)−C(17)	120.1(4)

Table 7.6 continued

C(15)−C(11)−C(12)−Ir(2)	59.3(3)
C(16)−C(11)−C(12)−Ir(2)	−118.4(4)
N(2)−Ir(2)−C(12)−C(11)	70.1(2)
C(15)−Ir(2)−C(12)−C(11)	−36.8(2)
C(13)−Ir(2)−C(12)−C(11)	−116.9(3)
C(14)−Ir(2)−C(12)−C(11)	−80.5(2)
Cl(1)−Ir(2)−C(12)−C(11)	−77.8(4)
Cl(2)−Ir(2)−C(12)−C(11)	160.46(19)
N(2)−Ir(2)−C(12)−C(13)	−173.0(2)
C(15)−Ir(2)−C(12)−C(13)	80.1(2)
C(11)−Ir(2)−C(12)−C(13)	116.9(3)
C(14)−Ir(2)−C(12)−C(13)	36.4(2)
Cl(1)−Ir(2)−C(12)−C(13)	39.1(4)
Cl(2)−Ir(2)−C(12)−C(13)	−82.6(2)
N(2)−Ir(2)−C(12)−C(17)	−51.5(4)
C(15)−Ir(2)−C(12)−C(17)	−158.3(4)
C(11)−Ir(2)−C(12)−C(17)	−121.5(4)
C(13)−Ir(2)−C(12)−C(17)	121.6(4)
C(14)−Ir(2)−C(12)−C(17)	158.0(4)
Cl(1)−Ir(2)−C(12)−C(17)	160.7(2)
Cl(2)−Ir(2)−C(12)−C(17)	38.9(3)
C(11)−C(12)−C(13)−C(14)	1.8(4)
C(17)−C(12)−C(13)−C(14)	179.7(4)
Ir(2)−C(12)−C(13)−C(14)	−60.1(3)
C(11)−C(12)−C(13)−C(18)	−178.9(3)
C(17)−C(12)−C(13)−C(18)	−1.1(6)
Ir(2)−C(12)−C(13)−C(18)	119.2(4)
C(11)−C(12)−C(13)−Ir(2)	61.9(2)
C(17)−C(12)−C(13)−Ir(2)	−120.2(4)
N(2)−Ir(2)−C(13)−C(14)	132.6(3)
C(12)−Ir(2)−C(13)−C(14)	119.6(3)
C(15)−Ir(2)−C(13)−C(14)	37.9(2)
C(11)−Ir(2)−C(13)−C(14)	81.1(2)
Cl(1)−Ir(2)−C(13)−C(14)	−45.8(2)
Cl(2)−Ir(2)−C(13)−C(14)	−138.4(2)
N(2)−Ir(2)−C(13)−C(12)	13.0(4)
C(15)−Ir(2)−C(13)−C(12)	−81.7(2)
C(11)−Ir(2)−C(13)−C(12)	−38.5(2)
C(14)−Ir(2)−C(13)−C(12)	−119.6(3)
Cl(1)−Ir(2)−C(13)−C(12)	−165.39(17)
Cl(2)−Ir(2)−C(13)−C(12)	102.0(2)
N(2)−Ir(2)−C(13)−C(18)	−106.1(4)
C(12)−Ir(2)−C(13)−C(18)	−119.1(4)
C(15)−Ir(2)−C(13)−C(18)	159.2(4)

Table 7.6 continued

C(11)−Ir(2)−C(13)−C(18)	−157.6(3)
C(14)−Ir(2)−C(13)−C(18)	121.3(4)
Cl(1)−Ir(2)−C(13)−C(18)	75.5(3)
Cl(2)−Ir(2)−C(13)−C(18)	−17.1(3)
C(12)−C(13)−C(14)−C(15)	−0.2(4)
C(18)−C(13)−C(14)−C(15)	−179.4(3)
Ir(2)−C(13)−C(14)−C(15)	−59.4(2)
C(12)−C(13)−C(14)−C(19)	179.3(3)
C(18)−C(13)−C(14)−C(19)	0.0(6)
Ir(2)−C(13)−C(14)−C(19)	120.0(4)
C(12)−C(13)−C(14)−Ir(2)	59.3(3)
C(18)−C(13)−C(14)−Ir(2)	−120.0(4)
N(2)−Ir(2)−C(14)−C(13)	−126.3(3)
C(12)−Ir(2)−C(14)−C(13)	−37.3(2)
C(15)−Ir(2)−C(14)−C(13)	−118.9(3)
C(11)−Ir(2)−C(14)−C(13)	−80.6(2)
Cl(1)−Ir(2)−C(14)−C(13)	143.6(2)
Cl(2)−Ir(2)−C(14)−C(13)	50.4(2)
N(2)−Ir(2)−C(14)−C(15)	−7.4(4)
C(12)−Ir(2)−C(14)−C(15)	81.6(2)
C(11)−Ir(2)−C(14)−C(15)	38.2(2)
C(13)−Ir(2)−C(14)−C(15)	118.9(3)
Cl(1)−Ir(2)−C(14)−C(15)	−97.50(19)
Cl(2)−Ir(2)−C(14)−C(15)	169.24(16)
N(2)−Ir(2)−C(14)−C(19)	112.4(4)
C(12)−Ir(2)−C(14)−C(19)	−158.5(4)
C(15)−Ir(2)−C(14)−C(19)	119.9(4)
C(11)−Ir(2)−C(14)−C(19)	158.1(4)
C(13)−Ir(2)−C(14)−C(19)	−121.2(4)
Cl(1)−Ir(2)−C(14)−C(19)	22.4(3)
Cl(2)−Ir(2)−C(14)−C(19)	−70.9(3)
C(12)−C(11)−C(15)−C(14)	2.6(4)
C(16)−C(11)−C(15)−C(14)	−179.7(4)
Ir(2)−C(11)−C(15)−C(14)	61.8(2)
C(12)−C(11)−C(15)−C(20)	−180.0(3)
C(16)−C(11)−C(15)−C(20)	−2.3(6)
Ir(2)−C(11)−C(15)−C(20)	−120.8(4)
C(12)−C(11)−C(15)−Ir(2)	−59.2(3)
C(16)−C(11)−C(15)−Ir(2)	118.5(4)
C(13)−C(14)−C(15)−C(11)	−1.5(4)
C(19)−C(14)−C(15)−C(11)	179.0(3)
Ir(2)−C(14)−C(15)−C(11)	−61.8(2)
C(13)−C(14)−C(15)−C(20)	−178.9(3)
C(19)−C(14)−C(15)−C(20)	1.6(6)

Table 7.6 continued

Ir(2)−C(14)−C(15)−C(20)	120.8(4)
C(13)−C(14)−C(15)−Ir(2)	60.3(3)
C(19)−C(14)−C(15)−Ir(2)	−119.2(4)
N(2)−Ir(2)−C(15)−C(11)	−66.7(2)
C(12)−Ir(2)−C(15)−C(11)	36.9(2)
C(13)−Ir(2)−C(15)−C(11)	80.2(2)
C(14)−Ir(2)−C(15)−C(11)	117.0(3)
Cl(1)−Ir(2)−C(15)−C(11)	−155.75(18)
Cl(2)−Ir(2)−C(15)−C(11)	90.6(3)
N(2)−Ir(2)−C(15)−C(14)	176.29(18)
C(12)−Ir(2)−C(15)−C(14)	−80.1(2)
C(11)−Ir(2)−C(15)−C(14)	−117.0(3)
C(13)−Ir(2)−C(15)−C(14)	−36.7(2)
Cl(1)−Ir(2)−C(15)−C(14)	87.28(19)
Cl(2)−Ir(2)−C(15)−C(14)	−26.4(4)
N(2)−Ir(2)−C(15)−C(20)	55.7(3)
C(12)−Ir(2)−C(15)−C(20)	159.3(4)
C(11)−Ir(2)−C(15)−C(20)	122.4(4)
C(13)−Ir(2)−C(15)−C(20)	−157.3(4)
C(14)−Ir(2)−C(15)−C(20)	−120.6(4)
Cl(1)−Ir(2)−C(15)−C(20)	−33.3(3)
Cl(2)−Ir(2)−C(15)−C(20)	−147.0(2)
C(25)−Sn(1)−C(21)−C(22)	−72.8(5)
Cl(4)−Sn(1)−C(21)−C(22)	144.0(3)
Cl(3)−Sn(1)−C(21)−C(22)	44.1(3)
Sn(1)−C(21)−C(22)−C(23)	−179.7(3)
C(21)−C(22)−C(23)−C(24)	−175.3(3)
C(21)−Sn(1)−C(25)−C(26)	−169.6(3)
Cl(4)−Sn(1)−C(25)−C(26)	−26.8(3)
Cl(3)−Sn(1)−C(25)−C(26)	72.9(3)
Sn(1)−C(25)−C(26)−C(27)	179.8(3)
C(25)−C(26)−C(27)−C(28)	175.2(4)
C(33)#1−C(31)−C(32)−C(34)	175.4(11)
C(33)#1−C(31)−C(32)−C(33)	−1.3(15)
C(34)−C(32)−C(33)−C(31)#1	−176.0(9)
C(31)−C(32)−C(33)−C(31)#1	1.1(13)

Symmetry transformations used to generate equivalent atoms: $\#1\ -x,\ -y+2,\ -z$

8 Full X-ray data of S_3N_2O

Table 8.1 Crystal data and structure refinement for S_3N_2O

Identification code	vmdw2	
Empirical formula	N2 O S3	
Formula weight	140.2	
Temperature	93(2) K	
Wavelength	0.710 73 Å	
Crystal system	Monoclinic	
Space group	Cc	
Unit cell dimensions	a = 7.617(5) Å	$\alpha = 90°$
	b = 9.230(6) Å	$\beta = 115.920(6)°$
	c = 7.050(5) Å	$\gamma = 90°$
Volume	445.7(5) Å^3	
Z	4	
Density (calculated)	2.089 Mg/^{3}m	
Absorption coefficient	1.497 mm^{-1}	
F(000)	280	
Crystal size	0.1000 × 0.0300 × 0.0300 mm^3	
Theta range for data collection	6.98 to 36.62°	
Index ranges	$-12 \leq h \leq 6, -15 \leq k \leq 15, -6 \leq l \leq 11$	
Reflections collected	3792	
Independent reflections	993 [R(int) = 0.0324]	
Completeness to theta = 36.62°	70.4 %	
Absorption correction	Multiscan	
Max. and min. transmission	1.0000 and 0.3400	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	993 / 2 / 56	
Goodness-of-fit on F^2	1.054	
Final R indices [I>2sigma(I)]	R1 = 0.0215, wR2 = 0.0533	
R indices (all data)	R1 = 0.0229, wR2 = 0.0537	
Absolute structure parameter	0.45(10)	
Largest diff. peak and hole	0.336 and −0.258 e·Å^{-3}	

Table 8.2 Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for S_3N_2O. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
S(2)	7037(1)	-2575(1)	3281(1)	18(1)
N(3)	7217(3)	-1150(1)	1994(3)	21(1)
S(4)	8680(1)	-1262(1)	979(1)	22(1)
N(5)	9605(2)	-2833(2)	1395(3)	21(1)
S(1)	8527(1)	-4135(1)	2085(1)	15(1)
O(1)	6964(2)	-4770(1)	168(3)	22(1)

Table 8.3 Bond lengths [Å] and angles [°] for S_3N_2O

S(2)−N(3)	1.6372(18)
S(2)−S(1)	2.2158(9)
N(3)−S(4)	1.5689(19)
S(4)−N(5)	1.5827(18)
N(5)−S(1)	1.6447(16)
S(1)−O(1)	1.4769(17)
N(3)−S(2)−S(1)	97.49(7)
S(4)−N(3)−S(2)	116.63(9)
N(3)−S(4)−N(5)	108.85(8)
S(4)−N(5)−S(1)	119.03(10)
O(1)−S(1)−N(5)	109.05(10)
O(1)−S(1)−S(2)	105.30(7)
N(5)−S(1)−S(2)	92.43(7)

Symmetry transformations used to generate equivalent atoms:

Table 8.4 Anisotropic displacement parameters ($Å^2 \times 10^3$) for S_3N_2O. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2\ a^{*2}\ U^{11} + \ldots + 2\ h\ k\ a^*\ b^*\ U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
S(2)	20(1)	18(1)	19(1)	-1(1)	11(1)	2(1)
N(3)	20(1)	15(1)	24(1)	0(1)	5(1)	2(1)
S(4)	20(1)	20(1)	24(1)	6(1)	7(1)	-4(1)
N(5)	18(1)	24(1)	25(1)	4(1)	13(1)	0(1)
S(1)	15(1)	14(1)	17(1)	0(1)	7(1)	1(1)
O(1)	23(1)	22(1)	22(1)	-6(1)	9(1)	-2(1)

Table 8.5 Torsion angles [°] for S_3N_2O

S(1)−S(2)−N(3)−S(4)	−14.31(12)
S(2)−N(3)−S(4)−N(5)	2.39(15)
N(3)−S(4)−N(5)−S(1)	17.43(15)
S(4)−N(5)−S(1)−O(1)	84.44(14)
S(4)−N(5)−S(1)−S(2)	−22.66(12)
N(3)−S(2)−S(1)−O(1)	−90.40(10)
N(3)−S(2)−S(1)−N(5)	20.11(10)

Symmetry transformations used to generate equivalent atoms: