ORGANOMETALLICS
Organometallics, 1998, 17(24), 5384-5389, DOI:10.1021/om980683f

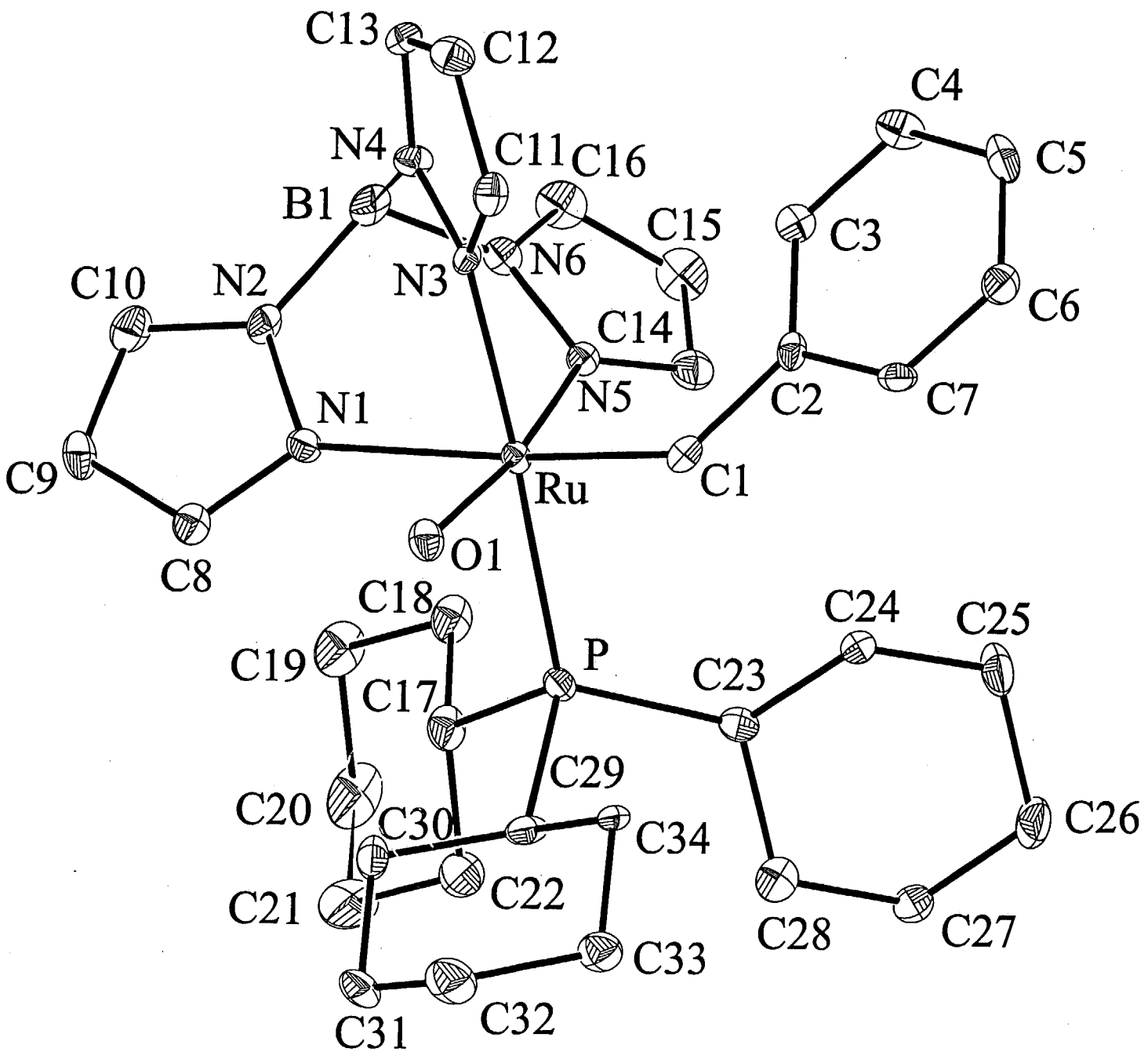

Table 1. Crystal data and structure refinement for MSS12.

Empirical formula	$C_{40.50}H_{65.75}B_2F_4N_6O_{2.88}PRu$
Formula weight	912.40
Crystallization Solvent	Et_2O/acetone
Crystal Habit	Flake
Crystal size	.30 x .26 x .04 mm^3
Crystal color	Emerald green

Data Collection

Type of diffractometer	CAD-4	
Wavelength	0.71073 Å MoKα	
Data Collection Temperature	85 K	
Theta range for reflections used in lattice determination	12 to 15°	
Unit cell dimensions	a = 20.195(5) Å b = 10.629(3) Å c = 21.205(7) Å	α= 90° β= 91.14(2)° γ = 90°
Volume	4551(2) $Å^3$	
Z	4	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Density (calculated)	1.332 Mg/m^3	
F(000)	1915	
Theta range for data collection	1.5 to 22.5°	
Completeness to theta = 22.5°	100.0 %	
Index ranges	-21<=h<=21, -11<=k<=10, 0<=l<=22	
Data collection scan type	Ω–scans	
Reflections collected	13603	
Independent reflections	5952 [R_{int}= 0.0381; GOF_{merge}=0.96]	
Absorption coefficient	0.438 mm^{-1}	
Absorption correction	None	
Number of standards	3 reflections measured every 75min.	
Variation of standards	Within counting statistics.	

Table 1 (cont.)

Structure solution and Refinement

Structure solution program	SHELXS-97 (Sheldrick, 1990)
Primary solution method	direct methods
Secondary solution method	difference map
Hydrogen placement	difference map/geometrical
Structure refinement program	SHELXL-97 (Sheldrick, 1997)
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5952 / 0 / 695
Treatment of hydrogen atoms	mixed
Goodness-of-fit on F^2	1.322
Final R indices [$I>2\sigma(I)$]	R1 = 0.0446, wR2 = 0.0714
R indices (all data)	R1 = 0.0694, wR2 = 0.0780
Type of weighting scheme used	calculated
Weighting scheme used	$w=1/\sigma^2(F_o^2)$
Max shift/error	0.022
Average shift/error	0.001
Largest diff. peak and hole	0.560 and -0.421 e.Å^{-3}

Special Refinement Details

Ψ-scans showed that no absorption correction was needed.

A background function of θ was used; based on backgrounds of reflections with $I<8\sigma(I)$.

The diethyl ether solvent is slightly disordered and partially present; it refined to a population of 0.872(5). The hydrogen atoms on the ether were placed at calculated positions; the coordinates of all other hydrogen atoms were refined. The U_{iso}'s of all hydrogen atoms were fixed at 120% of the U_{eq} of the attached atom.

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for MSS12. U_{eq} is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Ru	6919(1)	4277(1)	3358(1)	9(1)
C1	7055(2)	3520(4)	2571(2)	9(1)
C2	6860(2)	2327(4)	2280(2)	12(1)
C3	6563(2)	1341(4)	2618(2)	13(1)
C4	6392(2)	242(4)	2319(2)	16(1)
C5	6504(2)	77(5)	1682(2)	17(1)
C6	6794(2)	1035(4)	1346(2)	16(1)
C7	6965(2)	2138(4)	1637(2)	12(1)
O1	6608(2)	5915(3)	2842(1)	14(1)
B1	6032(3)	3232(5)	4470(2)	15(1)
N1	6606(2)	5252(3)	4217(2)	12(1)
N2	6209(2)	4607(3)	4619(2)	13(1)
C8	6642(2)	6420(5)	4448(2)	15(1)
C9	6273(2)	6545(5)	4985(2)	16(1)
C10	6007(2)	5374(5)	5078(2)	19(1)
N3	5910(2)	3692(3)	3323(2)	10(1)
N4	5636(2)	3186(3)	3847(2)	12(1)
C11	5458(2)	3563(4)	2857(2)	13(1)
C12	4898(2)	2990(4)	3078(2)	17(1)
C13	5028(2)	2764(4)	3704(2)	13(1)
N5	7099(2)	2719(3)	3909(2)	10(1)
N6	6672(2)	2452(3)	4382(2)	13(1)
C14	7567(2)	1822(5)	3941(2)	18(1)
C15	7438(2)	990(5)	4425(2)	21(1)
C16	6872(2)	1418(5)	4696(2)	20(1)
P	8030(1)	5022(1)	3426(1)	12(1)
C17	8282(2)	5485(5)	4246(2)	17(1)
C18	8160(2)	4461(5)	4735(2)	18(1)
C19	8273(2)	4972(6)	5408(2)	24(1)
C20	8965(3)	5520(6)	5491(2)	33(2)
C21	9086(3)	6540(6)	5010(3)	32(2)
C22	8981(2)	6025(5)	4340(2)	22(1)
C23	8714(2)	3918(4)	3187(2)	13(1)
C24	8534(2)	2965(4)	2667(2)	14(1)
C25	9079(2)	1992(5)	2577(3)	22(1)
C26	9737(2)	2603(5)	2431(3)	23(1)
C27	9919(2)	3588(5)	2927(2)	18(1)
C28	9364(2)	4549(5)	3001(2)	17(1)
C29	8213(2)	6452(4)	2965(2)	14(1)
C30	7893(2)	7687(5)	3193(2)	16(1)
C31	8137(3)	8792(5)	2808(3)	21(1)
C32	8018(3)	8602(5)	2106(2)	24(1)
C33	8316(2)	7395(5)	1874(2)	18(1)
C34	8061(2)	6270(4)	2257(2)	13(1)
O2	5957(2)	7884(3)	3340(1)	16(1)
C35	5367(3)	9180(6)	4040(3)	36(2)
C36	5479(2)	8002(5)	3672(2)	16(1)
C37	4986(3)	6954(6)	3739(3)	32(2)

O3	9666(2)	4303(4)	799(2)	35(1)
C38	8631(3)	3372(8)	788(3)	64(3)
C39	9005(3)	4479(7)	907(3)	45(2)
C40	10039(3)	5393(7)	915(3)	53(2)
C41	10762(3)	5098(8)	779(3)	67(3)
B2	6491(2)	5718(6)	1170(2)	16(1)
F1	7085(1)	5129(2)	1060(1)	21(1)
F2	6171(1)	5118(2)	1679(1)	21(1)
F3	6591(1)	6966(2)	1338(1)	24(1)
F4	6073(1)	5643(2)	640(1)	19(1)

Table 3. Bond lengths [Å] and angles [°] for MSS12.

Ru-C1	1.878(4)	P-C23	1.889(4)
Ru-N5	2.056(4)	C17-C18	1.526(6)
Ru-N3	2.129(3)	C17-C22	1.533(6)
Ru-O1	2.143(3)	C17-H17	0.94(4)
Ru-N1	2.200(4)	C18-C19	1.541(6)
Ru-P	2.3822(13)	C18-H18A	1.00(4)
C1-C2	1.460(6)	C18-H18B	0.98(4)
C1-H1	0.93(4)	C19-C20	1.521(7)
C2-C7	1.400(6)	C19-H19A	0.98(5)
C2-C3	1.409(6)	C19-H19B	1.07(5)
C3-C4	1.369(6)	C20-C21	1.511(8)
C3-H3	0.91(4)	C20-H20A	0.95(5)
C4-C5	1.386(6)	C20-H20B	0.89(5)
C4-H4	0.91(4)	C21-C22	1.533(7)
C5-C6	1.380(7)	C21-H21A	0.97(5)
C5-H5	0.92(5)	C21-H21B	0.92(5)
C6-C7	1.366(6)	C22-H22A	0.98(5)
C6-H6	0.85(4)	C22-H22B	1.05(5)
C7-H7	0.92(4)	C23-C28	1.533(6)
O1-H1O	0.70(4)	C23-C24	1.535(6)
O1-H2O	0.86(4)	C23-H23	0.97(4)
B1-N4	1.531(6)	C24-C25	1.526(6)
B1-N2	1.536(7)	C24-H24A	0.95(4)
B1-N6	1.550(6)	C24-H24B	0.96(4)
B1-H1B	1.09(4)	C25-C26	1.515(7)
N1-C8	1.336(6)	C25-H25A	0.91(5)
N1-N2	1.367(5)	C25-H25B	0.93(5)
N2-C10	1.340(6)	C26-C27	1.525(7)
C8-C9	1.380(6)	C26-H26A	0.99(5)
C8-H8	0.91(4)	C26-H26B	0.91(5)
C9-C10	1.371(7)	C27-C28	1.527(6)
C9-H9	0.82(4)	C27-H27A	1.02(4)
C10-H10	0.87(4)	C27-H27B	0.95(4)
N3-C11	1.339(5)	C28-H28A	0.98(4)
N3-N4	1.362(5)	C28-H28B	0.89(4)
N4-C13	1.336(5)	C29-C34	1.539(6)
C11-C12	1.376(6)	C29-C30	1.545(6)
C11-H11	0.87(4)	C29-H29	0.94(4)
C12-C13	1.369(6)	C30-C31	1.518(7)
C12-H12	0.89(4)	C30-H30A	0.98(4)
C13-H13	0.94(4)	C30-H30B	0.90(4)
N5-C14	1.342(6)	C31-C32	1.518(7)
N5-N6	1.365(5)	C31-H31A	0.96(4)
N6-C16	1.343(6)	C31-H31B	0.95(5)
C14-C15	1.384(7)	C32-C33	1.504(7)
C14-H14	0.93(4)	C32-H32A	0.96(5)
C15-C16	1.367(7)	C32-H32B	1.06(5)
C15-H15	0.88(5)	C33-C34	1.540(6)
C16-H16	0.90(4)	C33-H33A	0.92(4)
P-C29	1.848(5)	C33-H33B	0.98(4)
P-C17	1.869(4)	C34-H34A	0.98(4)

C34-H34B	1.00(4)	C3-C4-H4	120(3)
O2-C36	1.213(5)	C5-C4-H4	119(3)
C35-C36	1.494(7)	C6-C5-C4	119.3(5)
C35-H35A	1.03(5)	C6-C5-H5	125(3)
C35-H35B	1.03(5)	C4-C5-H5	116(3)
C35-H35C	0.78(5)	C7-C6-C5	120.4(4)
C36-C37	1.503(7)	C7-C6-H6	118(3)
C37-H37A	0.95(5)	C5-C6-H6	121(3)
C37-H37B	0.95(5)	C6-C7-C2	121.4(4)
C37-H37C	0.94(5)	C6-C7-H7	123(3)
O3-C39	1.372(7)	C2-C7-H7	115(3)
O3-C40	1.402(7)	Ru-O1-H1O	109(4)
C38-C39	1.418(9)	Ru-O1-H2O	114(3)
C38-H38A	0.9800	H1O-O1-H2O	108(5)
C38-H38B	0.9800	N4-B1-N2	108.9(4)
C38-H38C	0.9800	N4-B1-N6	107.6(4)
C39-H39A	0.9900	N2-B1-N6	110.0(4)
C39-H39B	0.9900	N4-B1-H1B	111(2)
C40-C41	1.526(9)	N2-B1-H1B	108(2)
C40-H40A	0.9900	N6-B1-H1B	111(2)
C40-H40B	0.9900	C8-N1-N2	105.4(4)
C41-H41A	0.9800	C8-N1-Ru	136.7(3)
C41-H41B	0.9800	N2-N1-Ru	117.5(3)
C41-H41C	0.9800	C10-N2-N1	109.8(4)
B2-F1	1.376(6)	C10-N2-B1	131.0(4)
B2-F3	1.386(6)	N1-N2-B1	119.1(3)
B2-F4	1.394(5)	N1-C8-C9	111.4(4)
B2-F2	1.422(6)	N1-C8-H8	117(3)
		C9-C8-H8	131(3)
C1-Ru-N5	97.65(16)	C10-C9-C8	104.5(4)
C1-Ru-N3	90.04(16)	C10-C9-H9	130(3)
N5-Ru-N3	86.73(13)	C8-C9-H9	126(3)
C1-Ru-O1	86.65(16)	N2-C10-C9	108.8(4)
N5-Ru-O1	172.48(13)	N2-C10-H10	123(3)
N3-Ru-O1	87.09(13)	C9-C10-H10	128(3)
C1-Ru-N1	170.95(16)	C11-N3-N4	106.2(3)
N5-Ru-N1	87.64(13)	C11-N3-Ru	133.9(3)
N3-Ru-N1	82.91(13)	N4-N3-Ru	119.5(3)
O1-Ru-N1	87.34(13)	C13-N4-N3	109.6(3)
C1-Ru-P	92.40(14)	C13-N4-B1	131.9(4)
N5-Ru-P	94.45(10)	N3-N4-B1	118.5(3)
N3-Ru-P	177.12(10)	N3-C11-C12	110.3(4)
O1-Ru-P	91.53(9)	N3-C11-H11	119(3)
N1-Ru-P	94.51(10)	C12-C11-H11	130(3)
C2-C1-Ru	134.8(3)	C13-C12-C11	105.4(4)
C2-C1-H1	108(2)	C13-C12-H12	124(3)
Ru-C1-H1	117(2)	C11-C12-H12	130(3)
C7-C2-C3	117.5(4)	N4-C13-C12	108.5(4)
C7-C2-C1	119.4(4)	N4-C13-H13	122(3)
C3-C2-C1	123.1(4)	C12-C13-H13	130(3)
C4-C3-C2	120.4(4)	C14-N5-N6	105.7(4)
C4-C3-H3	115(3)	C14-N5-Ru	135.8(3)
C2-C3-H3	124(3)	N6-N5-Ru	118.5(3)
C3-C4-C5	120.9(5)	C16-N6-N5	110.2(4)

C16-N6-B1	128.5(4)
N5-N6-B1	121.2(4)
N5-C14-C15	110.4(4)
N5-C14-H14	119(3)
C15-C14-H14	130(3)
C16-C15-C14	105.6(4)
C16-C15-H15	123(3)
C14-C15-H15	131(3)
N6-C16-C15	108.1(4)
N6-C16-H16	124(3)
C15-C16-H16	128(3)
C29-P-C17	102.9(2)
C29-P-C23	102.4(2)
C17-P-C23	103.1(2)
C29-P-Ru	116.03(15)
C17-P-Ru	112.47(15)
C23-P-Ru	118.05(14)
C18-C17-C22	109.8(4)
C18-C17-P	113.5(3)
C22-C17-P	116.9(3)
C18-C17-H17	106(3)
C22-C17-H17	107(3)
P-C17-H17	102(3)
C17-C18-C19	110.7(4)
C17-C18-H18A	108(2)
C19-C18-H18A	107(3)
C17-C18-H18B	112(3)
C19-C18-H18B	109(2)
H18A-C18-H18B	109(4)
C20-C19-C18	111.1(4)
C20-C19-H19A	114(3)
C18-C19-H19A	110(3)
C20-C19-H19B	108(2)
C18-C19-H19B	109(2)
H19A-C19-H19B	104(3)
C21-C20-C19	110.9(5)
C21-C20-H20A	110(3)
C19-C20-H20A	111(3)
C21-C20-H20B	111(4)
C19-C20-H20B	108(3)
H20A-C20-H20B	106(4)
C20-C21-C22	110.3(5)
C20-C21-H21A	109(3)
C22-C21-H21A	109(3)
C20-C21-H21B	113(3)
C22-C21-H21B	109(3)
H21A-C21-H21B	107(4)
C17-C22-C21	111.4(4)
C17-C22-H22A	113(3)
C21-C22-H22A	108(3)
C17-C22-H22B	109(2)
C21-C22-H22B	108(2)
H22A-C22-H22B	107(3)
C28-C23-C24	107.2(4)
C28-C23-P	115.6(3)
C24-C23-P	116.0(3)
C28-C23-H23	109(2)
C24-C23-H23	103(3)
P-C23-H23	105(2)
C25-C24-C23	112.1(4)
C25-C24-H24A	105(3)
C23-C24-H24A	109(3)
C25-C24-H24B	109(3)
C23-C24-H24B	112(3)
H24A-C24-H24B	109(4)
C26-C25-C24	111.9(4)
C26-C25-H25A	108(3)
C24-C25-H25A	112(3)
C26-C25-H25B	110(3)
C24-C25-H25B	109(3)
H25A-C25-H25B	106(4)
C25-C26-C27	110.7(4)
C25-C26-H26A	108(3)
C27-C26-H26A	113(3)
C25-C26-H26B	111(3)
C27-C26-H26B	105(3)
H26A-C26-H26B	110(4)
C26-C27-C28	111.3(4)
C26-C27-H27A	113(2)
C28-C27-H27A	107(3)
C26-C27-H27B	112(3)
C28-C27-H27B	107(3)
H27A-C27-H27B	107(4)
C27-C28-C23	111.6(4)
C27-C28-H28A	108(2)
C23-C28-H28A	112(2)
C27-C28-H28B	110(3)
C23-C28-H28B	107(3)
H28A-C28-H28B	109(4)
C34-C29-C30	109.7(4)
C34-C29-P	112.0(3)
C30-C29-P	116.4(3)
C34-C29-H29	108(3)
C30-C29-H29	101(3)
P-C29-H29	108(3)
C31-C30-C29	110.3(4)
C31-C30-H30A	110(3)
C29-C30-H30A	110(3)
C31-C30-H30B	107(3)
C29-C30-H30B	108(3)
H30A-C30-H30B	111(4)
C30-C31-C32	112.2(4)
C30-C31-H31A	112(3)
C32-C31-H31A	110(3)
C30-C31-H31B	107(3)
C32-C31-H31B	115(3)
H31A-C31-H31B	101(4)
C33-C32-C31	112.1(4)

C33-C32-H32A	113(3)
C31-C32-H32A	110(3)
C33-C32-H32B	111(2)
C31-C32-H32B	108(2)
H32A-C32-H32B	103(4)
C32-C33-C34	110.5(4)
C32-C33-H33A	111(3)
C34-C33-H33A	105(3)
C32-C33-H33B	112(3)
C34-C33-H33B	107(3)
H33A-C33-H33B	112(4)
C29-C34-C33	110.8(4)
C29-C34-H34A	109(2)
C33-C34-H34A	107(2)
C29-C34-H34B	114(2)
C33-C34-H34B	109(2)
H34A-C34-H34B	107(3)
C36-C35-H35A	108(3)
C36-C35-H35B	112(3)
H35A-C35-H35B	111(4)
C36-C35-H35C	106(5)
H35A-C35-H35C	118(5)
H35B-C35-H35C	101(5)
O2-C36-C35	121.3(5)
O2-C36-C37	121.0(5)
C35-C36-C37	117.7(5)
C36-C37-H37A	109(3)
C36-C37-H37B	110(3)
H37A-C37-H37B	117(4)
C36-C37-H37C	114(3)
H37A-C37-H37C	107(4)
H37B-C37-H37C	100(4)

C39-O3-C40	112.3(5)
C39-C38-H38A	109.5
C39-C38-H38B	109.5
H38A-C38-H38B	109.5
C39-C38-H38C	109.5
H38A-C38-H38C	109.5
H38B-C38-H38C	109.5
O3-C39-C38	111.9(6)
O3-C39-H39A	109.2
C38-C39-H39A	109.2
O3-C39-H39B	109.2
C38-C39-H39B	109.2
H39A-C39-H39B	107.9
O3-C40-C41	108.1(6)
O3-C40-H40A	110.1
C41-C40-H40A	110.1
O3-C40-H40B	110.1
C41-C40-H40B	110.1
H40A-C40-H40B	108.4
C40-C41-H41A	109.5
C40-C41-H41B	109.5
H41A-C41-H41B	109.5
C40-C41-H41C	109.5
H41A-C41-H41C	109.5
H41B-C41-H41C	109.5
F1-B2-F3	110.9(4)
F1-B2-F4	110.7(4)
F3-B2-F4	110.1(4)
F1-B2-F2	109.6(4)
F3-B2-F2	107.5(4)
F4-B2-F2	107.9(4)

Table 4. Anisotropic displacement parameters ($Å^2 x 10^3$) for MSS12. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ru	11(1)	10(1)	7(1)	-1(1)	-1(1)	0(1)
C1	8(2)	13(3)	7(2)	6(2)	-1(2)	4(2)
C2	10(2)	13(3)	12(3)	-3(2)	-1(2)	3(2)
C3	13(3)	15(3)	11(3)	1(2)	-2(2)	0(2)
C4	20(3)	15(3)	12(3)	5(2)	-4(2)	-3(2)
C5	19(3)	13(3)	19(3)	-6(2)	-4(2)	4(2)
C6	14(3)	21(3)	13(3)	-5(2)	0(2)	-2(2)
C7	9(2)	11(3)	16(3)	1(2)	1(2)	-2(2)
O1	15(2)	15(2)	12(2)	-3(2)	-1(1)	1(2)
B1	20(3)	19(3)	8(3)	4(2)	5(2)	-1(3)
N1	16(2)	12(2)	9(2)	-1(2)	2(2)	-3(2)
N2	15(2)	18(2)	6(2)	0(2)	2(2)	0(2)
C8	14(3)	18(3)	11(3)	-1(2)	-1(2)	1(2)
C9	20(3)	19(3)	10(3)	-6(2)	-2(2)	3(2)
C10	21(3)	23(3)	12(3)	2(2)	4(2)	1(2)
N3	9(2)	10(2)	10(2)	0(2)	3(2)	1(2)
N4	14(2)	13(2)	8(2)	2(2)	0(2)	-3(2)
C11	17(3)	16(3)	7(3)	0(2)	0(2)	2(2)
C12	15(3)	17(3)	18(3)	0(2)	-3(2)	-2(2)
C13	10(3)	14(3)	14(3)	0(2)	2(2)	-1(2)
N5	11(2)	12(2)	8(2)	-1(2)	-1(2)	0(2)
N6	16(2)	12(2)	10(2)	2(2)	-1(2)	0(2)
C14	15(3)	18(3)	19(3)	-2(2)	-3(2)	-2(2)
C15	23(3)	21(3)	20(3)	6(3)	-7(2)	5(2)
C16	27(3)	21(3)	12(3)	6(2)	-1(2)	-2(3)
P	12(1)	10(1)	13(1)	-2(1)	0(1)	-1(1)
C17	16(3)	20(3)	13(3)	-5(2)	-3(2)	1(2)
C18	18(3)	25(3)	13(3)	-4(2)	-2(2)	1(3)
C19	24(3)	37(3)	12(3)	-3(3)	-2(2)	0(3)
C20	25(3)	60(5)	14(3)	-15(3)	-5(2)	-1(3)
C21	21(3)	51(4)	25(3)	-16(3)	-4(3)	-14(3)
C22	20(3)	26(3)	19(3)	-7(2)	0(2)	-4(2)
C23	14(3)	12(3)	13(3)	2(2)	-1(2)	-2(2)
C24	14(3)	13(3)	15(3)	-1(2)	5(2)	-2(2)
C25	23(3)	16(3)	25(3)	-7(3)	0(3)	6(2)
C26	15(3)	23(3)	30(3)	-9(3)	3(2)	6(2)
C27	10(3)	19(3)	27(3)	-5(2)	1(2)	0(2)
C28	15(3)	22(3)	13(3)	-1(2)	-2(2)	1(2)
C29	12(3)	16(3)	14(3)	1(2)	2(2)	-5(2)
C30	13(3)	18(3)	16(3)	-6(2)	0(2)	3(2)
C31	21(3)	8(3)	35(3)	-2(2)	5(3)	-1(2)
C32	27(3)	15(3)	31(3)	5(3)	2(3)	0(3)
C33	17(3)	14(3)	21(3)	4(2)	1(2)	0(2)
C34	10(3)	9(3)	20(3)	0(2)	6(2)	-2(2)
O2	22(2)	12(2)	14(2)	3(2)	3(2)	4(2)
C35	41(4)	39(4)	28(3)	-10(3)	7(3)	13(3)
C36	14(3)	26(3)	6(2)	3(2)	-5(2)	7(2)
C37	28(3)	50(4)	19(3)	-2(3)	4(3)	-10(3)

O3	34(3)	44(3)	28(2)	1(2)	5(2)	-4(2)
C38	45(5)	115(8)	31(4)	3(5)	-8(4)	-35(5)
C39	39(4)	61(5)	35(4)	-3(4)	1(3)	-12(4)
C40	69(5)	41(5)	48(5)	-9(4)	-14(4)	-8(4)
C41	43(5)	103(7)	54(5)	11(5)	-6(4)	-26(5)
B2	20(3)	15(3)	14(3)	-1(3)	2(2)	0(3)
F1	22(2)	23(2)	19(2)	-3(1)	0(1)	6(1)
F2	29(2)	21(2)	12(1)	3(1)	1(1)	-2(1)
F3	36(2)	12(2)	23(2)	-3(1)	-3(1)	1(1)
F4	26(1)	21(2)	10(1)	1(1)	-4(1)	-4(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for MSS12.

	x	y	z	U_{iso}
H1	7248(18)	4020(40)	2262(18)	11
H3	6440(20)	1390(40)	3030(20)	16
H4	6200(20)	-390(40)	2540(20)	19
H5	6370(20)	-680(40)	1510(20)	20
H6	6850(20)	970(40)	950(20)	19
H7	7150(20)	2810(40)	1427(19)	15
H1O	6440(20)	5730(50)	2570(20)	17
H2O	6360(20)	6410(40)	3050(20)	17
H1B	5741(19)	2860(40)	4857(19)	18
H8	6910(20)	6970(40)	4250(20)	17
H9	6250(20)	7170(40)	5210(20)	19
H10	5740(20)	5140(40)	5370(20)	22
H11	5550(20)	3820(40)	2480(20)	16
H12	4520(20)	2800(40)	2880(20)	20
H13	4760(20)	2380(40)	4010(20)	15
H14	7920(20)	1860(40)	3670(20)	21
H15	7670(20)	360(40)	4580(20)	26
H16	6640(20)	1050(40)	5000(20)	24
H17	7980(20)	6140(40)	4330(20)	20
H18A	8490(20)	3770(40)	4670(20)	22
H18B	7710(20)	4110(40)	4697(19)	22
H19A	8170(20)	4320(50)	5720(20)	29
H19B	7920(20)	5700(50)	5490(20)	29
H20A	9290(20)	4880(50)	5460(20)	39
H20B	9000(20)	5820(50)	5880(20)	39
H21A	9540(20)	6830(50)	5060(20)	39
H21B	8820(20)	7230(50)	5060(20)	39
H22A	9080(20)	6690(40)	4040(20)	26
H22B	9330(20)	5310(40)	4270(20)	26
H23	8800(20)	3390(40)	3550(20)	16
H24A	8500(20)	3390(40)	2270(20)	17
H24B	8130(20)	2540(40)	2750(20)	17
H25A	8980(20)	1440(40)	2260(20)	26
H25B	9120(20)	1510(40)	2940(20)	26
H26A	9700(20)	2950(40)	2000(20)	27
H26B	10070(20)	2030(40)	2450(20)	27
H27A	10330(20)	4080(40)	2820(19)	22
H27B	10000(20)	3220(40)	3330(20)	22
H28A	9510(20)	5160(40)	3320(20)	20
H28B	9290(20)	4950(40)	2640(20)	20
H29	8670(20)	6640(40)	3015(19)	17
H30A	8000(20)	7820(40)	3640(20)	19
H30B	7450(20)	7630(40)	3130(20)	19
H31A	8600(20)	8970(40)	2890(20)	26
H31B	7940(20)	9520(40)	2980(20)	26
H32A	8170(20)	9320(50)	1880(20)	29
H32B	7500(20)	8620(40)	2010(20)	29

H33A	8770(20)	7390(40)	1940(20)	21
H33B	8190(20)	7230(40)	1430(20)	21
H34A	7580(20)	6250(40)	2191(19)	15
H34B	8243(19)	5480(40)	2077(19)	15
H35A	5700(20)	9850(50)	3890(20)	43
H35B	4890(20)	9500(50)	3990(20)	43
H35C	5380(30)	8980(60)	4390(20)	43
H37A	5120(20)	6260(50)	3490(20)	39
H37B	4920(20)	6790(50)	4170(20)	39
H37C	4550(20)	7170(50)	3610(20)	39
H38A	8164	3532	874	77
H38B	8796	2693	1062	77
H38C	8677	3125	346	77
H39A	8835	5165	632	54
H39B	8948	4739	1351	54
H40A	9995	5656	1360	63
H40B	9879	6086	640	63
H41A	11032	5854	849	80
H41B	10800	4825	339	80
H41C	10919	4426	1060	80

Table 6. Torsion angles [°] for MSS12.

N5-Ru-C1-C2	43.5(4)	C11-N3-N4-B1	-178.2(4)
N3-Ru-C1-C2	-43.2(4)	Ru-N3-N4-B1	8.7(5)
O1-Ru-C1-C2	-130.3(4)	N2-B1-N4-C13	-120.7(5)
N1-Ru-C1-C2	-81.9(12)	N6-B1-N4-C13	120.1(5)
P-Ru-C1-C2	138.3(4)	N2-B1-N4-N3	56.6(5)
Ru-C1-C2-C7	170.3(3)	N6-B1-N4-N3	-62.6(5)
Ru-C1-C2-C3	-9.2(7)	N4-N3-C11-C12	0.4(5)
C7-C2-C3-C4	0.5(6)	Ru-N3-C11-C12	172.0(3)
C1-C2-C3-C4	180.0(4)	N3-C11-C12-C13	-0.3(5)
C2-C3-C4-C5	-0.2(7)	N3-N4-C13-C12	0.1(5)
C3-C4-C5-C6	0.1(7)	B1-N4-C13-C12	177.6(5)
C4-C5-C6-C7	-0.4(7)	C11-C12-C13-N4	0.1(5)
C5-C6-C7-C2	0.7(7)	C1-Ru-N5-C14	47.1(4)
C3-C2-C7-C6	-0.8(6)	N3-Ru-N5-C14	136.7(4)
C1-C2-C7-C6	179.7(4)	O1-Ru-N5-C14	171.6(8)
C1-Ru-N1-C8	-88.9(12)	N1-Ru-N5-C14	-140.2(4)
N5-Ru-N1-C8	145.1(5)	P-Ru-N5-C14	-45.9(4)
N3-Ru-N1-C8	-127.9(5)	C1-Ru-N5-N6	-134.1(3)
O1-Ru-N1-C8	-40.5(5)	N3-Ru-N5-N6	-44.5(3)
P-Ru-N1-C8	50.8(4)	O1-Ru-N5-N6	-9.6(12)
C1-Ru-N1-N2	82.3(11)	N1-Ru-N5-N6	38.6(3)
N5-Ru-N1-N2	-43.7(3)	P-Ru-N5-N6	132.9(3)
N3-Ru-N1-N2	43.3(3)	C14-N5-N6-C16	0.0(5)
O1-Ru-N1-N2	130.7(3)	Ru-N5-N6-C16	-179.1(3)
P-Ru-N1-N2	-138.0(3)	C14-N5-N6-B1	-175.7(4)
C8-N1-N2-C10	0.5(5)	Ru-N5-N6-B1	5.2(5)
Ru-N1-N2-C10	-173.2(3)	N4-B1-N6-C16	-118.9(5)
C8-N1-N2-B1	176.7(4)	N2-B1-N6-C16	122.6(5)
Ru-N1-N2-B1	3.0(5)	N4-B1-N6-N5	56.0(5)
N4-B1-N2-C10	112.3(5)	N2-B1-N6-N5	-62.5(5)
N6-B1-N2-C10	-130.0(5)	N6-N5-C14-C15	0.3(5)
N4-B1-N2-N1	-62.9(5)	Ru-N5-C14-C15	179.2(3)
N6-B1-N2-N1	54.7(5)	N5-C14-C15-C16	-0.5(5)
N2-N1-C8-C9	-0.6(5)	N5-N6-C16-C15	-0.3(5)
Ru-N1-C8-C9	171.3(3)	B1-N6-C16-C15	175.0(4)
N1-C8-C9-C10	0.4(6)	C14-C15-C16-N6	0.5(5)
N1-N2-C10-C9	-0.3(5)	C1-Ru-P-C29	79.1(2)
B1-N2-C10-C9	-175.9(4)	N5-Ru-P-C29	176.94(19)
C8-C9-C10-N2	-0.1(5)	N3-Ru-P-C29	-69(2)
C1-Ru-N3-C11	-35.0(4)	O1-Ru-P-C29	-7.63(18)
N5-Ru-N3-C11	-132.6(4)	N1-Ru-P-C29	-95.08(19)
O1-Ru-N3-C11	51.7(4)	C1-Ru-P-C17	-162.9(2)
N1-Ru-N3-C11	139.4(4)	N5-Ru-P-C17	-65.0(2)
P-Ru-N3-C11	113(2)	N3-Ru-P-C17	49(2)
C1-Ru-N3-N4	135.8(3)	O1-Ru-P-C17	110.40(19)
N5-Ru-N3-N4	38.2(3)	N1-Ru-P-C17	22.9(2)
O1-Ru-N3-N4	-137.5(3)	C1-Ru-P-C23	-43.0(2)
N1-Ru-N3-N4	-49.8(3)	N5-Ru-P-C23	54.85(19)
P-Ru-N3-N4	-76(2)	N3-Ru-P-C23	169(2)
C11-N3-N4-C13	-0.3(5)	O1-Ru-P-C23	-129.72(19)
Ru-N3-N4-C13	-173.4(3)	N1-Ru-P-C23	142.83(19)

C29-P-C17-C18	178.2(3)	C23-C24-C25-C26	-56.7(6)
C23-P-C17-C18	-75.5(4)	C24-C25-C26-C27	53.3(6)
Ru-P-C17-C18	52.7(4)	C25-C26-C27-C28	-54.1(6)
C29-P-C17-C22	-52.3(4)	C26-C27-C28-C23	58.5(5)
C23-P-C17-C22	53.9(4)	C24-C23-C28-C27	-58.8(5)
Ru-P-C17-C22	-177.8(3)	P-C23-C28-C27	170.1(3)
C22-C17-C18-C19	56.0(5)	C17-P-C29-C34	178.2(3)
P-C17-C18-C19	-171.0(3)	C23-P-C29-C34	71.5(4)
C17-C18-C19-C20	-56.4(6)	Ru-P-C29-C34	-58.6(3)
C18-C19-C20-C21	56.8(6)	C17-P-C29-C30	-54.5(4)
C19-C20-C21-C22	-57.0(6)	C23-P-C29-C30	-161.3(3)
C18-C17-C22-C21	-57.1(6)	Ru-P-C29-C30	68.7(4)
P-C17-C22-C21	171.7(4)	C34-C29-C30-C31	-56.9(5)
C20-C21-C22-C17	57.6(6)	P-C29-C30-C31	174.7(3)
C29-P-C23-C28	29.2(4)	C29-C30-C31-C32	55.5(5)
C17-P-C23-C28	-77.4(4)	C30-C31-C32-C33	-55.1(6)
Ru-P-C23-C28	157.9(3)	C31-C32-C33-C34	55.0(6)
C29-P-C23-C24	-97.6(4)	C30-C29-C34-C33	57.9(5)
C17-P-C23-C24	155.9(3)	P-C29-C34-C33	-171.3(3)
Ru-P-C23-C24	31.2(4)	C32-C33-C34-C29	-57.0(5)
C28-C23-C24-C25	57.8(5)	C40-O3-C39-C38	-180.0(6)
P-C23-C24-C25	-171.3(3)	C39-O3-C40-C41	-179.8(5)

Table 7. Hydrogen bonds for MSS12[Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O1-H2O...O2	0.86(4)	1.87(4)	2.697(5)	161(4)
O1-H1O...F2	0.70(4)	2.05(4)	2.738(4)	166(5)