

ORGANOMETALLICS

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Table 1. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 10. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
B(1)	7861(1)	492(1)	6143(1)	17(1)
N(1)	7872(1)	573(1)	5404(1)	20(1)
S(1)	7840(1)	-298(1)	7423(1)	20(1)
Ru(1)	6675(1)	595(1)	7006(1)	15(1)
C(1)	8047(1)	1202(1)	6712(1)	18(1)
C(2)	8234(1)	2132(1)	6688(1)	22(1)
C(3)	8422(1)	2610(2)	7267(1)	27(1)
C(4)	8447(1)	2207(2)	7925(1)	29(1)
C(5)	8272(1)	1336(2)	7991(1)	25(1)
C(6)	8062(1)	839(1)	7395(1)	20(1)
C(7)	7624(1)	-343(1)	6536(1)	18(1)
C(8)	7889(1)	1438(1)	5067(1)	23(1)
C(9)	8842(2)	1737(2)	4903(1)	31(1)
C(10)	7305(2)	1495(2)	4425(1)	31(1)
C(11)	8014(2)	-195(1)	4956(1)	24(1)
C(12)	7175(2)	-750(2)	4880(1)	37(1)
C(13)	8817(2)	-750(2)	5174(1)	32(1)
C(14)	5497(1)	961(1)	6442(1)	21(1)
C(15)	5310(1)	197(1)	6851(1)	21(1)
C(16)	5424(1)	438(1)	7563(1)	20(1)
C(17)	5678(1)	1339(1)	7595(1)	21(1)
C(18)	5731(1)	1661(1)	6904(1)	21(1)
C(19)	5382(2)	1039(2)	5681(1)	35(1)
C(20)	4960(2)	-657(2)	6581(2)	34(1)
C(21)	5269(2)	-146(2)	8170(1)	32(1)
C(22)	5845(2)	1869(2)	8233(1)	36(1)
C(23)	5945(2)	2585(2)	6694(2)	37(1)

Table 2. Bond lengths [Å] and angles [deg] for 10.

B(1)-N(1)	1.443(3)
B(1)-C(7)	1.523(3)
B(1)-C(1)	1.570(3)
B(1)-Ru(1)	2.449(2)
N(1)-C(8)	1.470(3)
N(1)-C(11)	1.472(3)
S(1)-C(7)	1.758(2)
S(1)-C(6)	1.761(2)
S(1)-Ru(1)	2.3566(5)
Ru(1)-C(14)	2.152(2)
Ru(1)-C(15)	2.156(2)
Ru(1)-C(18)	2.160(2)
Ru(1)-C(16)	2.180(2)
Ru(1)-C(17)	2.196(2)
Ru(1)-C(7)	2.213(2)
Ru(1)-C(6)	2.243(2)
Ru(1)-C(1)	2.326(2)
C(1)-C(6)	1.439(3)
C(1)-C(2)	1.442(3)
C(2)-C(3)	1.370(3)
C(3)-C(4)	1.419(3)
C(4)-C(5)	1.354(3)
C(5)-C(6)	1.420(3)
C(8)-C(10)	1.529(3)
C(8)-C(9)	1.533(3)
C(11)-C(12)	1.522(3)
C(11)-C(13)	1.530(3)
C(14)-C(15)	1.435(3)
C(14)-C(18)	1.437(3)
C(14)-C(19)	1.496(3)
C(15)-C(16)	1.441(3)
C(15)-C(20)	1.496(3)
C(16)-C(17)	1.423(3)
C(16)-C(21)	1.496(3)
C(17)-C(18)	1.433(3)
C(17)-C(22)	1.502(3)
C(18)-C(23)	1.497(3)
N(1)-B(1)-C(7)	124.9(2)
N(1)-B(1)-C(1)	129.9(2)
C(7)-B(1)-C(1)	105.1(2)
N(1)-B(1)-Ru(1)	133.28(14)
C(7)-B(1)-Ru(1)	62.70(10)
C(1)-B(1)-Ru(1)	66.59(10)
B(1)-N(1)-C(8)	121.4(2)
B(1)-N(1)-C(11)	121.7(2)
C(8)-N(1)-C(11)	116.2(2)
C(7)-S(1)-C(6)	92.43(9)
C(7)-S(1)-Ru(1)	63.11(6)
C(6)-S(1)-Ru(1)	64.13(6)
C(14)-Ru(1)-C(15)	38.93(8)
C(14)-Ru(1)-C(18)	38.92(8)
C(15)-Ru(1)-C(18)	64.90(8)
C(14)-Ru(1)-C(16)	64.86(7)
C(15)-Ru(1)-C(16)	38.83(7)
C(18)-Ru(1)-C(16)	64.15(7)
C(14)-Ru(1)-C(17)	64.81(7)
C(15)-Ru(1)-C(17)	64.58(7)
C(18)-Ru(1)-C(17)	38.39(8)
C(16)-Ru(1)-C(17)	37.94(7)
C(14)-Ru(1)-C(7)	118.91(7)

C(15)-Ru(1)-C(7)	111.85(7)
C(18)-Ru(1)-C(7)	150.06(7)
C(16)-Ru(1)-C(7)	133.51(7)
C(17)-Ru(1)-C(7)	170.08(7)
C(14)-Ru(1)-C(6)	152.85(8)
C(15)-Ru(1)-C(6)	166.78(8)
C(18)-Ru(1)-C(6)	120.93(7)
C(16)-Ru(1)-C(6)	130.42(7)
C(17)-Ru(1)-C(6)	111.71(7)
C(7)-Ru(1)-C(6)	69.51(7)
C(14)-Ru(1)-C(1)	119.87(7)
C(15)-Ru(1)-C(1)	156.47(7)
C(18)-Ru(1)-C(1)	105.03(7)
C(16)-Ru(1)-C(1)	158.00(7)
C(17)-Ru(1)-C(1)	121.76(7)
C(7)-Ru(1)-C(1)	65.47(7)
C(6)-Ru(1)-C(1)	36.65(7)
C(14)-Ru(1)-S(1)	158.85(6)
C(15)-Ru(1)-S(1)	126.18(6)
C(18)-Ru(1)-S(1)	161.68(6)
C(16)-Ru(1)-S(1)	113.83(5)
C(17)-Ru(1)-S(1)	128.43(6)
C(7)-Ru(1)-S(1)	45.11(5)
C(6)-Ru(1)-S(1)	44.93(5)
C(1)-Ru(1)-S(1)	69.96(5)
C(14)-Ru(1)-B(1)	105.23(7)
C(15)-Ru(1)-B(1)	125.14(7)
C(18)-Ru(1)-B(1)	117.40(7)
C(16)-Ru(1)-B(1)	163.35(7)
C(17)-Ru(1)-B(1)	152.14(7)
C(7)-Ru(1)-B(1)	37.70(7)
C(6)-Ru(1)-B(1)	64.48(7)
C(1)-Ru(1)-B(1)	38.27(7)
S(1)-Ru(1)-B(1)	70.19(5)
C(6)-C(1)-C(2)	113.7(2)
C(6)-C(1)-B(1)	113.0(2)
C(2)-C(1)-B(1)	133.3(2)
C(6)-C(1)-Ru(1)	68.56(10)
C(2)-C(1)-Ru(1)	124.65(13)
B(1)-C(1)-Ru(1)	75.13(11)
C(3)-C(2)-C(1)	122.2(2)
C(2)-C(3)-C(4)	121.1(2)
C(5)-C(4)-C(3)	120.2(2)
C(4)-C(5)-C(6)	119.0(2)
C(5)-C(6)-C(1)	123.6(2)
C(5)-C(6)-S(1)	122.6(2)
C(1)-C(6)-S(1)	113.68(14)
C(5)-C(6)-Ru(1)	124.74(14)
C(1)-C(6)-Ru(1)	74.78(11)
S(1)-C(6)-Ru(1)	70.94(7)
B(1)-C(7)-S(1)	114.64(14)
B(1)-C(7)-Ru(1)	79.61(11)
S(1)-C(7)-Ru(1)	71.78(7)
N(1)-C(8)-C(10)	113.9(2)
N(1)-C(8)-C(9)	112.1(2)
C(10)-C(8)-C(9)	110.3(2)
N(1)-C(11)-C(12)	112.2(2)
N(1)-C(11)-C(13)	112.8(2)
C(12)-C(11)-C(13)	111.8(2)
C(15)-C(14)-C(18)	107.5(2)
C(15)-C(14)-C(19)	126.2(2)
C(18)-C(14)-C(19)	126.0(2)
C(15)-C(14)-Ru(1)	70.67(11)
C(18)-C(14)-Ru(1)	70.84(11)
C(19)-C(14)-Ru(1)	128.3(2)

C(14)-C(15)-C(16)	107.7(2)
C(14)-C(15)-C(20)	125.1(2)
C(16)-C(15)-C(20)	126.9(2)
C(14)-C(15)-Ru(1)	70.40(11)
C(16)-C(15)-Ru(1)	71.49(11)
C(20)-C(15)-Ru(1)	128.8(2)
C(17)-C(16)-C(15)	108.5(2)
C(17)-C(16)-C(21)	125.3(2)
C(15)-C(16)-C(21)	126.1(2)
C(17)-C(16)-Ru(1)	71.65(11)
C(15)-C(16)-Ru(1)	69.67(11)
C(21)-C(16)-Ru(1)	126.23(14)
C(16)-C(17)-C(18)	107.6(2)
C(16)-C(17)-C(22)	126.7(2)
C(18)-C(17)-C(22)	125.7(2)
C(16)-C(17)-Ru(1)	70.41(11)
C(18)-C(17)-Ru(1)	69.44(11)
C(22)-C(17)-Ru(1)	126.5(2)
C(17)-C(18)-C(14)	108.6(2)
C(17)-C(18)-C(23)	126.0(2)
C(14)-C(18)-C(23)	125.2(2)
C(17)-C(18)-Ru(1)	72.17(11)
C(14)-C(18)-Ru(1)	70.24(11)
C(23)-C(18)-Ru(1)	126.1(2)

Symmetry transformations used to generate equivalent atoms:

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

	U11	U22	U33	U23	U13	U12
B(1)	15(1)	19(1)	18(1)	-1(1)	0(1)	2(1)
N(1)	24(1)	20(1)	16(1)	0(1)	1(1)	1(1)
S(1)	20(1)	23(1)	18(1)	4(1)	0(1)	5(1)
Ru(1)	13(1)	16(1)	16(1)	1(1)	0(1)	1(1)
C(1)	12(1)	21(1)	19(1)	0(1)	0(1)	1(1)
C(2)	16(1)	23(1)	27(1)	-1(1)	2(1)	-1(1)
C(3)	19(1)	24(1)	38(1)	-9(1)	-2(1)	-3(1)
C(4)	21(1)	39(1)	27(1)	-14(1)	-3(1)	0(1)
C(5)	18(1)	38(1)	20(1)	-6(1)	-2(1)	2(1)
C(6)	15(1)	24(1)	20(1)	-2(1)	-1(1)	2(1)
C(7)	20(1)	18(1)	16(1)	0(1)	0(1)	1(1)
C(8)	25(1)	23(1)	20(1)	3(1)	-1(1)	0(1)
C(9)	29(1)	32(1)	33(1)	6(1)	3(1)	-4(1)
C(10)	33(1)	37(1)	22(1)	10(1)	-3(1)	2(1)
C(11)	30(1)	25(1)	17(1)	-3(1)	2(1)	3(1)
C(12)	42(2)	39(1)	30(1)	-10(1)	-6(1)	-8(1)
C(13)	37(1)	30(1)	27(1)	-2(1)	6(1)	9(1)
C(14)	14(1)	28(1)	22(1)	1(1)	0(1)	2(1)
C(15)	14(1)	21(1)	28(1)	-2(1)	-1(1)	-1(1)
C(16)	13(1)	24(1)	24(1)	4(1)	1(1)	2(1)
C(17)	14(1)	25(1)	25(1)	-5(1)	1(1)	3(1)
C(18)	14(1)	18(1)	31(1)	2(1)	1(1)	3(1)
C(19)	27(1)	56(2)	23(1)	5(1)	-4(1)	8(1)
C(20)	24(1)	27(1)	51(2)	-10(1)	-3(1)	-4(1)
C(21)	21(1)	41(1)	35(1)	15(1)	4(1)	1(1)
C(22)	29(1)	44(2)	33(1)	-17(1)	-1(1)	7(1)
C(23)	26(1)	21(1)	63(2)	10(1)	4(1)	4(1)

Table 4. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 10

	x	y	z	U(eq)
H(2)	8215(16)	2433(16)	6250(13)	29(7)
H(3)	8558(17)	3191(17)	7239(13)	28(6)
H(4)	8583(17)	2546(18)	8308(14)	36(7)
H(5)	8287(17)	1054(18)	8395(15)	37(7)
H(7)	7457(14)	-900(15)	6380(11)	15(5)
H(8)	7638(15)	1844(14)	5390(11)	18(6)
H(9A)	8863(18)	2342(18)	4700(13)	35(7)
H(9B)	9133(19)	1345(20)	4561(15)	47(8)
H(9C)	9217(16)	1712(17)	5305(13)	28(6)
H(10A)	7257(17)	2099(18)	4271(13)	36(7)
H(10B)	6722(19)	1306(18)	4517(14)	37(7)
H(10C)	7533(18)	1173(18)	4039(14)	37(7)
H(11)	8152(16)	33(16)	4520(13)	27(6)
H(12A)	7288(22)	-1238(22)	4571(17)	60(10)
H(12B)	6672(21)	-430(20)	4688(16)	52(9)
H(12C)	6965(19)	-981(20)	5282(16)	44(8)
H(13A)	8887(19)	-1255(20)	4862(15)	45(8)
H(13B)	8736(17)	-1014(17)	5619(14)	34(7)
H(13C)	9334(20)	-400(19)	5192(14)	42(8)
H(19A)	5701(22)	1525(23)	5509(17)	60(10)
H(19B)	4776(21)	1171(19)	5553(15)	48(8)
H(19C)	5532(20)	502(20)	5457(16)	48(9)
H(20A)	4343(21)	-618(18)	6487(15)	45(8)
H(20B)	5049(22)	-1139(23)	6895(16)	59(10)
H(20C)	5243(19)	-828(18)	6176(15)	38(8)
H(21A)	5412(21)	-728(20)	8073(15)	46(9)
H(21B)	4687(18)	-120(17)	8331(13)	30(7)
H(21C)	5650(21)	-6(20)	8538(16)	51(9)
H(22A)	5320(19)	2127(18)	8387(14)	38(7)
H(22B)	6294(25)	2321(24)	8169(17)	66(10)
H(22C)	6080(22)	1508(22)	8609(17)	60(10)
H(23A)	5421(23)	2937(22)	6672(17)	62(10)
H(23B)	6255(21)	2595(20)	6273(16)	53(9)
H(23C)	6333(23)	2858(22)	7025(16)	55(9)