

Table S23. Atomic coordinates and equivalent isotropic displacement parameter for 7a. Ueq is defined as one third of the trace of the orthogonalized Uij tensor.

atom	x	y	z	Ueq
Ru1	0.38177(3)	0.255387(16)	0.02402(3)	0.02993(14)
N1	0.7213(7)	0.1266(4)	-0.0549(10)	0.100(2)
N2	0.4159(11)	0.2193(5)	-0.4230(7)	0.118(3)
N3	0.5168(9)	0.4456(4)	-0.1701(9)	0.103(2)
N4	0.8303(5)	0.3655(4)	0.1870(8)	0.0847(18)
N5	0.2153(5)	0.2938(3)	-0.1539(4)	0.0463(9)
N6	0.2313(5)	0.1622(2)	-0.1514(4)	0.0468(8)
C1	0.3182(4)	0.3227(2)	0.2427(4)	0.0358(7)
C2	0.4779(5)	0.3215(3)	0.2924(5)	0.0395(8)
C3	0.5122(5)	0.2360(3)	0.2669(5)	0.0423(9)
C4	0.3702(5)	0.1828(2)	0.2059(4)	0.0383(8)
C5	0.2492(5)	0.2366(3)	0.1892(5)	0.0382(8)
C6	0.2371(6)	0.4008(3)	0.2621(6)	0.0524(11)
C7	0.5871(6)	0.3985(3)	0.3886(6)	0.0532(11)
C8	0.6662(6)	0.2059(4)	0.3257(7)	0.0625(13)
C9	0.3545(7)	0.0895(3)	0.1950(6)	0.0574(12)
C10	0.0813(6)	0.2075(4)	0.1458(7)	0.0582(13)
C11	0.5348(5)	0.2362(3)	-0.1211(6)	0.0480(10)
C12	0.5664(5)	0.3249(3)	-0.0213(6)	0.0470(10)
C13	0.6403(6)	0.1755(4)	-0.0819(8)	0.0640(15)
C14	0.4682(9)	0.2269(4)	-0.2905(7)	0.0779(18)
C15	0.5308(7)	0.3905(4)	-0.1092(8)	0.0670(15)
C16	0.7121(6)	0.3464(3)	0.0981(7)	0.0601(14)
C17	0.1548(6)	0.2154(3)	-0.2273(5)	0.0529(11)
C18	0.0183(9)	0.1877(5)	-0.3743(8)	0.091(2)
C19	0.1527(7)	0.3730(3)	-0.1816(6)	0.0596(12)
C20	-0.0074(10)	0.3775(6)	-0.1540(10)	0.099(3)
C21	0.1501(10)	0.3894(5)	-0.3440(8)	0.088(2)
C22	0.2288(7)	0.0695(3)	-0.2057(6)	0.0638(14)
C23	0.0742(9)	0.0221(4)	-0.2096(9)	0.087(2)
C24	0.2749(9)	0.0399(4)	-0.3568(8)	0.0819(19)

Table S24. Anisotropic displacement parameters for 7a. The anisotropic displacement factor exponent takes the form: $-2\pi^2[(ha^*)^2U_{11} + \dots + 2hka^*b^*U_{12}]$

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ru1	0.03158(19)	0.02998(19)	0.02853(19)	0.00793(12)	0.00857(12)	-0.00005(11)
N1	0.064(3)	0.061(3)	0.156(6)	-0.012(4)	0.024(4)	0.019(3)
N2	0.202(9)	0.114(5)	0.053(3)	0.021(3)	0.062(4)	0.023(5)
N3	0.131(6)	0.078(4)	0.124(5)	0.061(4)	0.050(5)	0.003(4)
N4	0.042(2)	0.072(3)	0.131(5)	-0.002(3)	0.032(3)	-0.008(2)
N5	0.059(2)	0.0454(19)	0.0319(16)	0.0159(15)	0.0017(15)	0.0085(17)
N6	0.056(2)	0.0397(18)	0.0380(18)	0.0064(14)	0.0057(16)	-0.0016(15)
C1	0.0422(19)	0.0364(19)	0.0311(17)	0.0073(14)	0.0147(15)	0.0036(15)
C2	0.045(2)	0.042(2)	0.0320(17)	0.0097(15)	0.0112(15)	0.0015(16)
C3	0.046(2)	0.041(2)	0.038(2)	0.0139(16)	0.0047(16)	0.0058(17)

C4	0.048(2)	0.0370(19)	0.0301(17)	0.0123(15)	0.0079(15)	0.0009(16)
C5	0.043(2)	0.040(2)	0.0355(18)	0.0119(16)	0.0172(16)	-0.0032(16)
C6	0.058(3)	0.047(2)	0.061(3)	0.013(2)	0.030(2)	0.015(2)
C7	0.054(3)	0.049(2)	0.047(2)	0.0003(19)	0.007(2)	-0.008(2)
C8	0.050(3)	0.058(3)	0.069(3)	0.018(2)	-0.005(2)	0.011(2)
C9	0.078(3)	0.041(2)	0.048(2)	0.0183(19)	0.004(2)	-0.002(2)
C10	0.045(2)	0.059(3)	0.076(3)	0.016(3)	0.027(2)	-0.005(2)
C11	0.052(2)	0.046(2)	0.051(2)	0.0075(19)	0.026(2)	0.0001(19)
C12	0.050(2)	0.040(2)	0.057(3)	0.0078(19)	0.030(2)	-0.0019(18)
C13	0.048(3)	0.054(3)	0.083(4)	-0.006(3)	0.026(3)	-0.003(2)
C14	0.119(5)	0.078(4)	0.057(3)	0.014(3)	0.058(4)	0.018(4)
C15	0.084(4)	0.055(3)	0.077(4)	0.021(3)	0.046(3)	-0.004(3)
C16	0.051(3)	0.048(3)	0.087(4)	0.004(2)	0.041(3)	-0.004(2)
C17	0.050(2)	0.062(3)	0.034(2)	0.0105(19)	-0.0085(18)	-0.001(2)
C18	0.092(5)	0.080(4)	0.065(4)	0.008(3)	-0.036(3)	0.004(4)
C19	0.075(3)	0.052(3)	0.050(3)	0.020(2)	0.006(2)	0.017(2)
C20	0.097(5)	0.110(6)	0.101(6)	0.038(5)	0.024(4)	0.060(5)
C21	0.119(6)	0.079(4)	0.068(4)	0.045(3)	0.004(4)	0.012(4)
C22	0.080(4)	0.046(3)	0.047(3)	0.004(2)	-0.006(2)	-0.011(2)
C23	0.097(5)	0.056(3)	0.090(5)	0.009(3)	0.008(4)	-0.029(3)
C24	0.106(5)	0.060(3)	0.066(4)	-0.002(3)	0.013(4)	0.008(3)

Table S25. Bond distances (Å) and angles (deg) for 7a

distances											
Ru1	C11	2.129(4)	N5	C19	1.476(6)	C12	C16	1.440(8)			
Ru1	C12	2.147(4)	C1	C2	1.407(6)	C12	C15	1.448(8)			
Ru1	C1	2.260(4)	C1	C5	1.434(5)	C12	C11	1.499(6)			
Ru1	C2	2.320(4)	C1	C6	1.503(6)	C17	C18	1.520(7)			
Ru1	C3	2.272(4)	C2	C3	1.426(6)	C19	C21	1.519(8)			
Ru1	C4	2.210(4)	C2	C7	1.507(6)	C19	C20	1.545(10)			
Ru1	C5	2.189(4)	C3	C8	1.508(6)	C22	C24	1.507(9)			
Ru1	N5	2.108(3)	C4	C3	1.427(6)	C22	C23	1.558(9)			
Ru1	N6	2.074(4)	C4	C9	1.495(6)	C13	N1	1.132(8)			
Ru1	C17	2.558(4)	C5	C4	1.439(6)	C14	N2	1.129(9)			
N6	C17	1.321(6)	C5	C10	1.500(6)	C15	N3	1.134(8)			
N6	C22	1.481(6)	C11	C13	1.443(8)	C16	N4	1.141(8)			
N5	C17	1.321(6)	C11	C14	1.444(8)						
angles											
N6	Ru1	N5	62.0(2)	N5	Ru1	C3	160.5(2)	N6	Ru1	C3	123.9(2)
N5	Ru1	C11	92.6(2)	N5	Ru1	C2	128.3(2)	N6	Ru1	C1	121.6(2)
N5	Ru1	C12	92.7(2)	N6	Ru1	C11	86.5(2)	N6	Ru1	C2	148.7(2)
N5	Ru1	C17	31.0(2)	N6	Ru1	C12	122.4(2)	C11	Ru1	C12	41.0(2)
N5	Ru1	C4	133.8(2)	N6	Ru1	C17	31.0(2)	C11	Ru1	C5	161.5(2)
N5	Ru1	C5	101.0(2)	N6	Ru1	C5	88.8(2)	C12	Ru1	C5	148.6(2)
N5	Ru1	C1	99.4(2)	N6	Ru1	C4	90.4(2)	C11	Ru1	C4	123.9(2)

C12	Ru1	C4	133.2(2)	C17	N6	C22	128.9(4)	C2	C3	C4	107.5(4)
C5	Ru1	C4	38.2(2)	C17	N6	Ru1	95.2(3)	C2	C3	C8	126.4(4)
C11	Ru1	C1	152.0(2)	C22	N6	Ru1	134.1(3)	C4	C3	C8	124.9(4)
C12	Ru1	C1	112.6(2)	C17	N5	C19	127.5(4)	C2	C3	Ru1	73.8(2)
C5	Ru1	C1	37.6(1)	C17	N5	Ru1	93.6(3)	C4	C3	Ru1	69.1(2)
C4	Ru1	C1	62.5(1)	C19	N5	Ru1	137.6(3)	C8	C3	Ru1	132.2(4)
C11	Ru1	C3	106.0(2)	C1	C5	C4	107.8(3)	N6	C17	N5	109.2(4)
C12	Ru1	C3	97.4(2)	C1	C5	C10	126.1(4)	N6	C17	C18	123.7(5)
C5	Ru1	C3	62.5(2)	C4	C5	C10	125.6(4)	N5	C17	C18	127.2(5)
C4	Ru1	C3	37.1(2)	C1	C5	Ru1	73.9(2)	N6	C17	Ru1	53.8(2)
C1	Ru1	C3	61.3(2)	C4	C5	Ru1	71.7(2)	N5	C17	Ru1	55.3(2)
C11	Ru1	C2	119.1(2)	C10	C5	Ru1	126.5(3)	C18	C17	Ru1	177.2(4)
C12	Ru1	C2	88.3(2)	C3	C4	C5	107.7(3)	C13	C11	C14	113.9(5)
C5	Ru1	C2	61.1(2)	C3	C4	C9	124.2(4)	C13	C11	C12	119.5(5)
C4	Ru1	C2	61.0(1)	C5	C4	C9	127.0(4)	C14	C11	C12	116.2(5)
C1	Ru1	C2	35.8(1)	C3	C4	Ru1	73.8(2)	C13	C11	Ru1	113.8(4)
C3	Ru1	C2	36.2(2)	C5	C4	Ru1	70.1(2)	C14	C11	Ru1	116.3(4)
C11	Ru1	C17	89.7(2)	C9	C4	Ru1	130.9(3)	C12	C11	Ru1	70.1(2)
C12	Ru1	C17	110.2(2)	C1	C2	C3	109.3(4)	N4	C16	C12	176.2(6)
C5	Ru1	C17	95.4(2)	C1	C2	C7	123.0(4)	N6	C22	C24	116.0(5)
C4	Ru1	C17	113.8(2)	C3	C2	C7	126.5(4)	N6	C22	C23	111.1(5)
C1	Ru1	C17	113.4(2)	C1	C2	Ru1	69.8(2)	C24	C22	C23	112.6(5)
C3	Ru1	C17	150.8(2)	C3	C2	Ru1	70.1(2)	N5	C19	C21	113.7(5)
C2	Ru1	C17	149.1(2)	C7	C2	Ru1	136.3(3)	N5	C19	C20	111.8(5)
C2	C1	C5	107.7(3)	C16	C12	C15	111.8(5)	C21	C19	C20	110.6(6)
C2	C1	C6	125.0(4)	C16	C12	C11	116.3(4)	N3	C15	C12	173.3(8)
C5	C1	C6	126.9(4)	C15	C12	C11	115.3(5)	N2	C14	C11	179.7(9)
C2	C1	Ru1	74.5(2)	C16	C12	Ru1	119.9(3)	N1	C13	C11	178.3(7)
C5	C1	Ru1	68.5(2)	C15	C12	Ru1	118.4(4)				
C6	C1	Ru1	128.0(3)	C11	C12	Ru1	68.8(2)				

Table S26. Torsion angles (deg) for 7a.

N6	Ru1	C1	C2	149.6(2)	N6	Ru1	C1	C6	-87.8(4)
N5	Ru1	C1	C2	-147.6(2)	N5	Ru1	C1	C6	-25.0(4)
C11	Ru1	C1	C2	-33.5(4)	C11	Ru1	C1	C6	89.1(5)
C12	Ru1	C1	C2	-50.7(3)	C12	Ru1	C1	C6	72.0(4)
C5	Ru1	C1	C2	116.6(3)	C5	Ru1	C1	C6	-120.8(5)
C4	Ru1	C1	C2	77.6(2)	C4	Ru1	C1	C6	-159.8(4)
C3	Ru1	C1	C2	35.4(2)	C3	Ru1	C1	C6	158.0(4)
C17	Ru1	C1	C2	-176.6(2)	C2	Ru1	C1	C6	122.6(5)
N6	Ru1	C1	C5	33.0(3)	C17	Ru1	C1	C6	-54.0(4)
N5	Ru1	C1	C5	95.8(3)	N5	Ru1	N6	C17	-0.5(3)
C11	Ru1	C1	C5	-150.1(4)	C11	Ru1	N6	C17	-95.3(3)
C12	Ru1	C1	C5	-167.2(3)	C12	Ru1	N6	C17	-74.6(4)
C4	Ru1	C1	C5	-39.0(2)	C5	Ru1	N6	C17	102.6(3)
C3	Ru1	C1	C5	-81.2(3)	C4	Ru1	N6	C17	140.7(3)
C2	Ru1	C1	C5	-116.6(3)	C1	Ru1	N6	C17	83.2(3)
C17	Ru1	C1	C5	66.8(3)	C3	Ru1	N6	C17	157.8(3)

C2	Ru1	N6	C17	117.9(4)	C17	Ru1	C5	C4	122.4(2)
N5	Ru1	N6	C22	164.8(5)	N6	Ru1	C5	C10	-29.1(4)
C11	Ru1	N6	C22	70.0(5)	N5	Ru1	C5	C10	32.1(4)
C12	Ru1	N6	C22	90.7(5)	C11	Ru1	C5	C10	-104.2(6)
C5	Ru1	N6	C22	-92.1(5)	C12	Ru1	C5	C10	146.3(4)
C4	Ru1	N6	C22	-54.0(5)	C4	Ru1	C5	C10	-121.2(5)
C1	Ru1	N6	C22	-111.5(5)	C1	Ru1	C5	C10	123.3(5)
C3	Ru1	N6	C22	-36.9(5)	C3	Ru1	C5	C10	-158.8(5)
C2	Ru1	N6	C22	-76.8(6)	C2	Ru1	C5	C10	160.0(5)
C17	Ru1	N6	C22	165.3(7)	C17	Ru1	C5	C10	1.2(4)
N6	Ru1	N5	C17	0.5(3)	C1	C5	C4	C3	-0.9(4)
C11	Ru1	N5	C17	85.1(3)	C10	C5	C4	C3	-173.0(4)
C12	Ru1	N5	C17	126.2(3)	Ru1	C5	C4	C3	64.7(3)
C5	Ru1	N5	C17	-82.2(3)	C1	C5	C4	C9	167.5(4)
C4	Ru1	N5	C17	-59.6(4)	C10	C5	C4	C9	-4.6(7)
C1	Ru1	N5	C17	-120.3(3)	Ru1	C5	C4	C9	-126.9(4)
C3	Ru1	N5	C17	-112.3(5)	C1	C5	C4	Ru1	-65.6(3)
C2	Ru1	N5	C17	-143.8(3)	C10	C5	C4	Ru1	122.3(4)
N6	Ru1	N5	C19	167.4(6)	N6	Ru1	C4	C3	156.2(3)
C11	Ru1	N5	C19	-108.0(5)	N5	Ru1	C4	C3	-153.9(3)
C12	Ru1	N5	C19	-66.9(5)	C11	Ru1	C4	C3	70.2(3)
C5	Ru1	N5	C19	84.7(5)	C12	Ru1	C4	C3	18.2(3)
C4	Ru1	N5	C19	107.4(5)	C5	Ru1	C4	C3	-116.2(3)
C1	Ru1	N5	C19	46.6(5)	C1	Ru1	C4	C3	-77.9(3)
C3	Ru1	N5	C19	54.6(8)	C2	Ru1	C4	C3	-37.2(2)
C2	Ru1	N5	C19	23.1(6)	C17	Ru1	C4	C3	177.0(2)
C17	Ru1	N5	C19	166.9(7)	N6	Ru1	C4	C5	-87.6(2)
C2	C1	C5	C4	-0.5(4)	N5	Ru1	C4	C5	-37.6(3)
C6	C1	C5	C4	-173.7(4)	C11	Ru1	C4	C5	-173.6(2)
Ru1	C1	C5	C4	64.2(3)	C12	Ru1	C4	C5	134.4(3)
C2	C1	C5	C10	171.5(4)	C1	Ru1	C4	C5	38.3(2)
C6	C1	C5	C10	-1.6(7)	C3	Ru1	C4	C5	116.2(3)
Ru1	C1	C5	C10	-123.8(4)	C2	Ru1	C4	C5	79.1(2)
C2	C1	C5	Ru1	-64.7(3)	C17	Ru1	C4	C5	-66.7(3)
C6	C1	C5	Ru1	122.1(4)	N6	Ru1	C4	C9	34.7(4)
N6	Ru1	C5	C1	-152.4(2)	N5	Ru1	C4	C9	84.6(5)
N5	Ru1	C5	C1	-91.2(2)	C11	Ru1	C4	C9	-51.3(5)
C11	Ru1	C5	C1	132.5(5)	C12	Ru1	C4	C9	-103.3(5)
C12	Ru1	C5	C1	23.0(4)	C5	Ru1	C4	C9	122.3(5)
C4	Ru1	C5	C1	115.5(3)	C1	Ru1	C4	C9	160.6(5)
C3	Ru1	C5	C1	77.9(2)	C3	Ru1	C4	C9	-121.5(5)
C2	Ru1	C5	C1	36.7(2)	C2	Ru1	C4	C9	-158.6(5)
C17	Ru1	C5	C1	-122.1(3)	C17	Ru1	C4	C9	55.5(5)
N6	Ru1	C5	C4	92.2(2)	C5	C1	C2	C3	1.8(4)
N5	Ru1	C5	C4	153.3(2)	C6	C1	C2	C3	175.1(4)
C11	Ru1	C5	C4	17.0(6)	Ru1	C1	C2	C3	-59.1(3)
C12	Ru1	C5	C4	-92.4(4)	C5	C1	C2	C7	-166.3(4)
C1	Ru1	C5	C4	-115.5(3)	C6	C1	C2	C7	7.0(6)
C3	Ru1	C5	C4	-37.6(2)	Ru1	C1	C2	C7	132.8(4)
C2	Ru1	C5	C4	-78.8(2)	C5	C1	C2	Ru1	60.9(3)

C6	C1	C2	Ru1	-125.8(4)	C2	Ru1	C12	C11	140.9(3)
N6	Ru1	C2	C1	-56.1(4)	C17	Ru1	C12	C11	-64.5(3)
N5	Ru1	C2	C1	42.3(3)	C1	C2	C3	C4	-2.3(5)
C11	Ru1	C2	C1	162.7(2)	C7	C2	C3	C4	165.3(4)
C12	Ru1	C2	C1	134.4(3)	Ru1	C2	C3	C4	-61.2(3)
C5	Ru1	C2	C1	-38.5(2)	C1	C2	C3	C8	-170.2(4)
C4	Ru1	C2	C1	-82.4(3)	C7	C2	C3	C8	-2.6(7)
C3	Ru1	C2	C1	-120.5(4)	Ru1	C2	C3	C8	130.9(5)
C17	Ru1	C2	C1	6.0(4)	C1	C2	C3	Ru1	58.9(3)
N6	Ru1	C2	C3	64.5(4)	C7	C2	C3	Ru1	-133.5(4)
N5	Ru1	C2	C3	162.9(3)	C5	C4	C3	C2	2.0(4)
C11	Ru1	C2	C3	-76.8(3)	C9	C4	C3	C2	-166.8(4)
C12	Ru1	C2	C3	-105.0(3)	Ru1	C4	C3	C2	64.3(3)
C5	Ru1	C2	C3	82.0(3)	C5	C4	C3	C8	170.1(4)
C4	Ru1	C2	C3	38.1(2)	C9	C4	C3	C8	1.3(7)
C1	Ru1	C2	C3	120.5(4)	Ru1	C4	C3	C8	-127.6(5)
C17	Ru1	C2	C3	126.6(3)	C5	C4	C3	Ru1	-62.3(3)
N6	Ru1	C2	C7	-173.2(4)	C9	C4	C3	Ru1	128.9(4)
N5	Ru1	C2	C7	-74.8(5)	N6	Ru1	C3	C2	-145.6(2)
C11	Ru1	C2	C7	45.6(5)	N5	Ru1	C3	C2	-44.0(6)
C12	Ru1	C2	C7	17.3(5)	C11	Ru1	C3	C2	117.8(3)
C5	Ru1	C2	C7	-155.6(5)	C12	Ru1	C3	C2	76.8(3)
C4	Ru1	C2	C7	160.5(5)	C5	Ru1	C3	C2	-77.8(3)
C1	Ru1	C2	C7	-117.1(5)	C4	Ru1	C3	C2	-116.5(4)
C3	Ru1	C2	C7	122.4(6)	C1	Ru1	C3	C2	-35.0(2)
C17	Ru1	C2	C7	-111.0(5)	C17	Ru1	C3	C2	-122.1(4)
N6	Ru1	C12	C16	-141.6(4)	N6	Ru1	C3	C4	-29.1(3)
N5	Ru1	C12	C16	160.2(4)	N5	Ru1	C3	C4	72.5(5)
C11	Ru1	C12	C16	-109.0(5)	C11	Ru1	C3	C4	-125.7(3)
C5	Ru1	C12	C16	43.9(6)	C12	Ru1	C3	C4	-166.7(3)
C4	Ru1	C12	C16	-14.1(5)	C5	Ru1	C3	C4	38.7(2)
C1	Ru1	C12	C16	58.9(4)	C1	Ru1	C3	C4	81.5(3)
C3	Ru1	C12	C16	-3.1(4)	C2	Ru1	C3	C4	116.5(4)
C2	Ru1	C12	C16	32.0(4)	C17	Ru1	C3	C4	-5.6(5)
C17	Ru1	C12	C16	-173.5(4)	N6	Ru1	C3	C8	89.6(5)
N6	Ru1	C12	C15	75.5(4)	N5	Ru1	C3	C8	-168.8(5)
N5	Ru1	C12	C15	17.3(4)	C11	Ru1	C3	C8	-7.0(5)
C11	Ru1	C12	C15	108.1(5)	C12	Ru1	C3	C8	-48.0(5)
C5	Ru1	C12	C15	-99.0(5)	C5	Ru1	C3	C8	157.4(5)
C4	Ru1	C12	C15	-157.0(4)	C4	Ru1	C3	C8	118.7(5)
C1	Ru1	C12	C15	-84.1(4)	C1	Ru1	C3	C8	-159.8(5)
C3	Ru1	C12	C15	-146.0(4)	C2	Ru1	C3	C8	-124.8(5)
C2	Ru1	C12	C15	-111.0(4)	C17	Ru1	C3	C8	113.1(5)
C17	Ru1	C12	C15	43.6(4)	C22	N6	C17	N5	-165.7(5)
N6	Ru1	C12	C11	-32.6(3)	Ru1	N6	C17	N5	0.8(5)
N5	Ru1	C12	C11	-90.8(3)	C22	N6	C17	C18	15.0(9)
C5	Ru1	C12	C11	152.9(3)	Ru1	N6	C17	C18	-178.6(6)
C4	Ru1	C12	C11	94.9(3)	C22	N6	C17	Ru1	-166.4(6)
C1	Ru1	C12	C11	167.8(3)	C19	N5	C17	N6	-169.7(5)
C3	Ru1	C12	C11	105.9(3)	Ru1	N5	C17	N6	-0.8(4)

C19	N5	C17	C18	9.7(10)	C1	Ru1	C11	C13	89.9(5)
Ru1	N5	C17	C18	178.6(6)	C3	Ru1	C11	C13	31.6(4)
C19	N5	C17	Ru1	-168.9(6)	C2	Ru1	C11	C13	68.2(4)
N5	Ru1	C17	N6	179.1(5)	C17	Ru1	C11	C13	-123.5(4)
C11	Ru1	C17	N6	83.6(3)	N6	Ru1	C11	C14	42.7(4)
C12	Ru1	C17	N6	119.9(3)	N5	Ru1	C11	C14	-19.0(4)
C5	Ru1	C17	N6	-78.6(3)	C12	Ru1	C11	C14	-110.2(5)
C4	Ru1	C17	N6	-43.8(4)	C5	Ru1	C11	C14	118.2(6)
C1	Ru1	C17	N6	-112.8(3)	C4	Ru1	C11	C14	130.8(4)
C3	Ru1	C17	N6	-40.1(5)	C1	Ru1	C11	C14	-134.6(4)
C2	Ru1	C17	N6	-116.7(4)	C3	Ru1	C11	C14	167.0(4)
N6	Ru1	C17	N5	-179.1(5)	C2	Ru1	C11	C14	-156.3(4)
C11	Ru1	C17	N5	-95.5(3)	C17	Ru1	C11	C14	11.9(4)
C12	Ru1	C17	N5	-59.2(3)	N6	Ru1	C11	C12	152.9(3)
C5	Ru1	C17	N5	102.3(3)	N5	Ru1	C11	C12	91.2(3)
C4	Ru1	C17	N5	137.1(3)	C5	Ru1	C11	C12	-131.6(5)
C1	Ru1	C17	N5	68.1(3)	C4	Ru1	C11	C12	-119.0(3)
C3	Ru1	C17	N5	140.8(4)	C1	Ru1	C11	C12	-24.5(5)
C2	Ru1	C17	N5	64.3(4)	C3	Ru1	C11	C12	-82.8(3)
N6	Ru1	C17	C18	26(10)	C2	Ru1	C11	C12	-46.1(3)
N5	Ru1	C17	C18	-155(10)	C17	Ru1	C11	C12	122.1(3)
C11	Ru1	C17	C18	109(10)	C15	C12	C16	N4	-34(9)
C12	Ru1	C17	C18	146(10)	C11	C12	C16	N4	101(9)
C5	Ru1	C17	C18	-53(10)	Ru1	C12	C16	N4	-180(100)
C4	Ru1	C17	C18	-18(10)	C17	N6	C22	C24	59.1(8)
C1	Ru1	C17	C18	-87(10)	Ru1	N6	C22	C24	-101.9(5)
C3	Ru1	C17	C18	-15(10)	C17	N6	C22	C23	-71.1(7)
C2	Ru1	C17	C18	-91(10)	Ru1	N6	C22	C23	127.8(5)
C16	C12	C11	C13	7.1(6)	C17	N5	C19	C21	-67.3(8)
C15	C12	C11	C13	140.7(5)	Ru1	N5	C19	C21	129.3(5)
Ru1	C12	C11	C13	-106.8(4)	C17	N5	C19	C20	58.9(7)
C16	C12	C11	C14	-135.8(5)	Ru1	N5	C19	C20	-104.6(6)
C15	C12	C11	C14	-2.1(7)	C16	C12	C15	N3	6(6)
Ru1	C12	C11	C14	110.3(5)	C11	C12	C15	N3	-130(6)
C16	C12	C11	Ru1	113.9(4)	Ru1	C12	C15	N3	152(6)
C15	C12	C11	Ru1	-112.4(4)	C13	C11	C14	N2	53(100)
N6	Ru1	C11	C13	-92.7(4)	C12	C11	C14	N2	-162(100)
N5	Ru1	C11	C13	-154.4(4)	Ru1	C11	C14	N2	-82(100)
C12	Ru1	C11	C13	114.4(5)	C14	C11	C13	N1	-23(24)
C5	Ru1	C11	C13	-17.2(8)	C12	C11	C13	N1	-166(24)
C4	Ru1	C11	C13	-4.6(4)	Ru1	C11	C13	N1	114(24)

Table S27. Least-squares planes data for 7a.

Least-squares planes (x,y,z in crystal coordinates) and deviations from them
 (* indicates atom used to define plane)

Plane 1 C₅-ring of η-C₅Me₅ moiety

$$-2.6802 (.0178) x - 3.4428 (.0304) y + 8.9014 (.0024) z = .2027 (.0100)$$

* -0.0066 (.0024) C1
 * .0119 (.0025) C2
 * -0.0125 (.0025) C3
 * .0084 (.0024) C4
 * -0.0012 (.0023) C5
 -1.8914 (.0018) Ru1
 Rms deviation of fitted atoms = .0091

Plane 2 Ru1-N5-N6-C17 plane

$$7.4514 (.0091) x + .7759 (.0450) y - 6.8405 (.0103) z = 2.8810 (.0106)$$

Angle to previous plane (with approximate esd) = 37.95 (.17)

* -0.0024 (.0014) Ru1
 * .0039 (.0022) N5
 * .0040 (.0023) N6
 * -0.0055 (.0032) C17
 Rms deviation of fitted atoms = .0041

Table S28. Hydrogen coordinates and isotropic displacement parameters ($\text{\AA}^2$) for 7a.

atom	x	y	z	U(eq)
H6A	0.1287	0.3855	0.2179	0.079
H6B	0.2717	0.4396	0.2073	0.079
H6C	0.2590	0.4272	0.3736	0.079
H7A	0.5348	0.4482	0.3863	0.080
H7B	0.6715	0.4031	0.3439	0.080
H7C	0.6247	0.3932	0.4971	0.080
H8A	0.6579	0.1454	0.2913	0.094
H8B	0.6997	0.2219	0.4402	0.094
H8C	0.7390	0.2312	0.2829	0.094
H9A	0.2487	0.0671	0.1505	0.086
H9B	0.3914	0.0789	0.2998	0.086
H9C	0.4133	0.0626	0.1278	0.086
H10A	0.0653	0.1469	0.1122	0.087
H10B	0.0275	0.2317	0.0604	0.087
H10C	0.0438	0.2253	0.2371	0.087
H18A	0.0011	0.1270	-0.4039	0.137
H18B	0.0385	0.2088	-0.4609	0.137
H18C	-0.0709	0.2099	-0.3510	0.137
H19	0.2209	0.4194	-0.1015	0.072
H20A	-0.0031	0.3685	-0.0498	0.149
H20B	-0.0791	0.3346	-0.2335	0.149
H20C	-0.0396	0.4322	-0.1615	0.149
H21A	0.2497	0.3847	-0.3605	0.133
H21B	0.1228	0.4453	-0.3484	0.133
H21C	0.0763	0.3486	-0.4259	0.133
H22	0.3064	0.0528	-0.1215	0.077
H23A	0.0500	0.0429	-0.1110	0.131
H23B	0.0829	-0.0375	-0.2232	0.131
H23C	-0.0056	0.0316	-0.2969	0.131

H24A	0.3718	0.0697	-0.3476	0.123
H24B	0.1988	0.0507	-0.4457	0.123
H24C	0.2834	-0.0198	-0.3734	0.123
