Supporting Information

Structural, Electronic and Acid/Base Properties of $[\text{Ru}(\text{bpy})_2(\text{bpy}(\text{OH})_2)]^{2+}$ (bpy = 2,2'-bipyridine, $\text{bpy}(\text{OH})_2$ = 4,4'-dihydroxy-2,2'-bipyridine)

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IR Spectroscopy

Figure S1 – FT-IR Spectrum of [Ru(bpy)₂(bpy(OMe)₂)]²⁺[PF₆]₂⁻

Figure S2 – FT-IR Spectrum of [Ru(bpy)₂(bpy(OH)₂)]²⁺[PF₆]₂⁻

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Figure S5 – Full ^1H -NMR Spectrum of $[\text{Ru}(\text{bpy})_2(\text{bpy}(\text{OH})_2)][\text{PF}_6]_2$

Figure S6 – Aromatic region of ^1H -NMR Spectrum of $[\text{Ru}(\text{bpy})_2(\text{bpy}(\text{OH})_2)][\text{PF}_6]_2$

Electrochemistry

Figure S7 – Cyclic Voltammogram of [Ru(bpy)₃][PF₆]₂ in acetonitrile with 0.1M tetrabutylammonium hexafluorophosphate. Potentials reported vs SCE.

Figure S8 – Cyclic Voltammogram of [Ru(bpy)₂(bpy(OMe)₂)] [PF₆]₂ in acetonitrile with 0.1M tetrabutylammonium hexafluorophosphate. Potentials reported vs SCE.

Figure S9 - Cyclic Voltammogram of $[\text{Ru}(\text{bpy})_2(\text{bpy}(\text{OH})_2)][\text{PF}_6]_2$ in acetonitrile with 0.1M tetrabutylammonium hexafluorophosphate. Data was collected with a platinum working electrode. Potentials reported vs SCE.

Absorbance Spectroscopy

Figure S10 - UV/Visible spectrum of $[\text{Ru}(\text{bpy})_3]^{2+}$ in water and (—) HCl; (—) NaOH.

Figure S11 - UV/Visible spectrum of $[\text{Ru}(\text{bpy})_2(\text{bpy}(\text{OMe})_2)]^{2+}$ in water and (—) HCl; (—) NaOH.

Table S1. UV/Visible Absorption Data for [Ru(bpy)₂(bpy(OH)₂)](PF₆)₂ in DCE

complex	energy (eV)	λ (nm)	ϵ (M ⁻¹ cm ⁻¹)
protonated	3.796	327	9410
	3.477	357(sh)	6400
	2.853	435(sh)	9800
	2.647	469	11200
deprotonated	3.557	349(sh)	10900
	3.232	384	11600
	2.652	468	5590
	2.324	534	8400

DCE = 1,2-dichloroethane

Table S2. UV/Visible Absorption Data for [Ru(bpy)₂(bpy(OH)₂)](PF₆)₂ in ACN

complex	energy (eV)	λ (nm)	ϵ (M ⁻¹ cm ⁻¹)
protonated	3.808	326	10000
	3.487	356(sh)	6810
	2.860	434(sh)	10700
	2.687	462	12100
deprotonated	3.506	354(sh)	11230
	3.275	379	12100
	2.664	466	6350
	2.360	526	8810

ACN = acetonitrile

Table S3. UV/Visible Absorption Data for [Ru(bpy)₂(bpy(OH)₂)](PF₆)₂ in EtOH

complex	energy (eV)	λ (nm)	ϵ (M ⁻¹ cm ⁻¹)
protonated	3.808	326	9140
	3.477	357(sh)	6410
	2.853	435(sh)	9650
	2.681	463	10700
deprotonated	3.672	338	9020
	3.292	377	11100
	2.722	456	6610
	2.429	511	8690

EtOH = ethanol

Table S4. UV/Visible Absorption Data for [Ru(bpy)₂(bpy(OH)₂)](PF₆)₂ in MeOH

complex	energy (eV)	λ (nm)	ϵ (M ⁻¹ cm ⁻¹)
protonated	3.796	327	9650
	3.467	358(sh)	6960
	2.827	439(sh)	10100
	2.669	465	10700
deprotonated	3.727	333	9640
	3.337	372	9920
	2.740	453	7510
	2.468	503	9280

MeOH = methanol

Crystallographic Data

Table S5. Crystal data and structure refinement for paul008.

Identification code	paul008	
Empirical formula	C48 H44 F12 N8 O3 P2 Ru	
Formula weight	1171.92	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 11.8349(8) Å	a = 90°.
	b = 28.306(2) Å	b = 93.195(2)°.
	c = 14.7157(10) Å	g = 90°.
Volume	4922.0(6) Å ³	
Z	4	
Density (calculated)	1.581 Mg/m ³	
Absorption coefficient	0.480 mm ⁻¹	
F(000)	2376	
Crystal size	0.27 x 0.24 x 0.04 mm ³	
Theta range for data collection	1.56 to 33.21°.	
Index ranges	-18<=h<=16, -38<=k<=43, -22<=l<=21	
Reflections collected	65664	
Independent reflections	18801 [R(int) = 0.0361]	
Completeness to theta = 33.21°	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9810 and 0.8812	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	18801 / 15 / 688	
Goodness-of-fit on F ²	1.029	
Final R indices [I>2sigma(I)]	R1 = 0.0535, wR2 = 0.1185	
R indices (all data)	R1 = 0.0818, wR2 = 0.1313	
Largest diff. peak and hole	1.319 and -1.117 e.Å ⁻³	

Table S6. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for paul008. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ru(1)	1311(1)	1787(1)	3426(1)	17(1)
P(1)	1221(1)	3152(1)	8523(1)	24(1)
F(1)	501(3)	3619(2)	8192(3)	35(1)
F(2)	2372(2)	3418(1)	8305(2)	48(1)
F(3)	1325(2)	3364(1)	9540(2)	54(1)
F(4)	74(2)	2910(1)	8763(2)	55(1)
F(5)	1127(2)	2962(1)	7520(2)	49(1)
F(6)	1932(3)	2706(1)	8867(2)	40(1)
F(1')	739(16)	3616(7)	8298(15)	35(1)
F(2')	1957(8)	3141(4)	7628(8)	48(1)
F(3')	2183(10)	3344(4)	9093(6)	54(1)
F(4')	495(9)	3059(4)	9383(9)	55(1)
F(5')	236(9)	2841(4)	7913(6)	49(1)
F(6')	1745(16)	2593(5)	8708(12)	40(1)
P(2)	6531(1)	894(1)	7127(1)	34(1)
F(7)	6419(2)	444(1)	7734(2)	62(1)
F(8)	6953(4)	1181(1)	7967(3)	146(2)
F(9)	5283(2)	1053(1)	7274(2)	62(1)
F(10)	6094(4)	604(1)	6271(2)	123(2)
F(11)	7777(2)	722(1)	6938(3)	104(1)
F(12)	6681(2)	1346(1)	6517(3)	123(2)
N(1)	483(2)	1771(1)	4621(1)	19(1)
N(2)	2060(2)	2344(1)	4127(1)	20(1)
N(3)	241(2)	2267(1)	2767(1)	20(1)
N(4)	2136(2)	1906(1)	2252(1)	20(1)
N(5)	2428(2)	1284(1)	3940(1)	21(1)
N(6)	590(2)	1178(1)	2894(1)	20(1)
O(1)	-972(2)	1823(1)	7102(2)	49(1)
O(2)	3384(2)	3422(1)	5730(2)	40(1)
C(1)	-361(2)	1473(1)	4818(2)	26(1)
C(2)	-880(2)	1475(1)	5632(2)	31(1)

C(3)	-513(2)	1795(1)	6290(2)	31(1)
C(4)	356(2)	2108(1)	6106(2)	27(1)
C(5)	826(2)	2092(1)	5264(2)	21(1)
C(6)	1713(2)	2421(1)	4982(2)	20(1)
C(7)	2156(2)	2779(1)	5527(2)	25(1)
C(8)	2986(2)	3074(1)	5190(2)	25(1)
C(9)	3340(2)	2998(1)	4322(2)	26(1)
C(10)	2864(2)	2632(1)	3820(2)	23(1)
C(11)	-741(2)	2432(1)	3064(2)	24(1)
C(12)	-1370(2)	2780(1)	2612(2)	29(1)
C(13)	-989(2)	2967(1)	1817(2)	29(1)
C(14)	7(2)	2795(1)	1492(2)	25(1)
C(15)	608(2)	2447(1)	1975(2)	20(1)
C(16)	1672(2)	2242(1)	1690(2)	21(1)
C(17)	2176(2)	2379(1)	902(2)	29(1)
C(18)	3172(2)	2163(1)	675(2)	33(1)
C(19)	3649(2)	1820(1)	1245(2)	32(1)
C(20)	3114(2)	1702(1)	2027(2)	26(1)
C(21)	3338(2)	1362(1)	4507(2)	26(1)
C(22)	4088(2)	1010(1)	4785(2)	34(1)
C(23)	3915(3)	559(1)	4441(2)	40(1)
C(24)	2986(3)	470(1)	3859(2)	36(1)
C(25)	2238(2)	836(1)	3631(2)	24(1)
C(26)	1186(2)	774(1)	3070(2)	24(1)
C(27)	770(3)	338(1)	2770(2)	32(1)
C(28)	-271(3)	309(1)	2303(2)	35(1)
C(29)	-877(2)	720(1)	2134(2)	32(1)
C(30)	-425(2)	1147(1)	2433(2)	26(1)
N(7)	1952(3)	1244(1)	6956(3)	68(1)
C(31)	2071(4)	870(2)	6682(3)	56(1)
C(32)	1475(3)	236(2)	5661(3)	55(1)
C(33)	1623(4)	-219(2)	5303(3)	56(1)
C(34)	2502(4)	-491(1)	5642(3)	51(1)
C(35)	3244(4)	-319(1)	6304(3)	53(1)
C(36)	3125(3)	121(1)	6646(2)	49(1)
C(37)	2218(3)	391(1)	6325(2)	41(1)

N(8)	2520(3)	190(1)	-1164(2)	55(1)
C(38)	3222(3)	335(1)	-669(2)	40(1)
C(39)	4935(3)	804(1)	-366(2)	42(1)
C(40)	5754(3)	984(1)	234(3)	53(1)
C(41)	5733(3)	884(2)	1155(3)	56(1)
C(42)	4886(3)	604(1)	1474(3)	53(1)
C(43)	4061(3)	421(1)	877(2)	41(1)
C(44)	4089(2)	523(1)	-41(2)	32(1)
O(3)	4948(2)	3920(1)	4943(2)	35(1)
C(45)	3638(3)	4508(2)	4412(3)	59(1)
C(46)	4774(4)	4325(2)	4397(4)	79(2)
C(47)	6112(3)	3787(1)	5085(2)	45(1)
C(48)	6592(4)	3583(2)	4243(3)	62(1)

Table S7. Bond lengths [$\text{\AA}$] and angles [$^\circ$] for paul008.

Ru(1)-N(6)	2.059(2)
Ru(1)-N(2)	2.058(2)
Ru(1)-N(4)	2.0590(19)
Ru(1)-N(5)	2.059(2)
Ru(1)-N(3)	2.061(2)
Ru(1)-N(1)	2.0611(18)
P(1)-F(1')	1.463(17)
P(1)-F(3')	1.478(11)
P(1)-F(5)	1.570(2)
P(1)-F(4)	1.579(2)
P(1)-F(6)	1.586(3)
P(1)-F(4')	1.591(10)
P(1)-F(2)	1.604(2)
P(1)-F(3)	1.610(2)
P(1)-F(2')	1.619(10)
P(1)-F(1)	1.632(3)
P(1)-F(5')	1.681(10)
P(1)-F(6')	1.718(15)
P(2)-F(8)	1.540(3)
P(2)-F(10)	1.566(3)
P(2)-F(7)	1.567(2)
P(2)-F(9)	1.570(2)
P(2)-F(12)	1.578(2)
P(2)-F(11)	1.592(2)
N(1)-C(1)	1.351(3)
N(1)-C(5)	1.356(3)
N(2)-C(10)	1.350(3)
N(2)-C(6)	1.362(3)
N(3)-C(11)	1.348(3)
N(3)-C(15)	1.365(3)
N(4)-C(20)	1.351(3)
N(4)-C(16)	1.357(3)
N(5)-C(21)	1.344(3)
N(5)-C(25)	1.360(3)

N(6)-C(30)	1.349(3)
N(6)-C(26)	1.361(3)
O(1)-C(3)	1.342(3)
O(2)-C(8)	1.335(3)
C(1)-C(2)	1.378(3)
C(2)-C(3)	1.378(4)
C(3)-C(4)	1.396(4)
C(4)-C(5)	1.387(3)
C(5)-C(6)	1.481(3)
C(6)-C(7)	1.378(3)
C(7)-C(8)	1.400(3)
C(8)-C(9)	1.383(3)
C(9)-C(10)	1.375(3)
C(11)-C(12)	1.382(4)
C(12)-C(13)	1.383(4)
C(13)-C(14)	1.385(4)
C(14)-C(15)	1.387(3)
C(15)-C(16)	1.469(3)
C(16)-C(17)	1.388(3)
C(17)-C(18)	1.385(4)
C(18)-C(19)	1.384(4)
C(19)-C(20)	1.385(3)
C(21)-C(22)	1.381(4)
C(22)-C(23)	1.385(5)
C(23)-C(24)	1.379(5)
C(24)-C(25)	1.392(4)
C(25)-C(26)	1.466(4)
C(26)-C(27)	1.393(4)
C(27)-C(28)	1.380(4)
C(28)-C(29)	1.381(4)
C(29)-C(30)	1.383(4)
N(7)-C(31)	1.142(5)
C(31)-C(37)	1.470(5)
C(32)-C(37)	1.351(5)
C(32)-C(33)	1.405(6)
C(33)-C(34)	1.366(6)

C(34)-C(35)	1.365(5)
C(35)-C(36)	1.354(5)
C(36)-C(37)	1.378(5)
N(8)-C(38)	1.149(4)
C(38)-C(44)	1.444(4)
C(39)-C(40)	1.371(5)
C(39)-C(44)	1.384(4)
C(40)-C(41)	1.386(6)
C(41)-C(42)	1.379(6)
C(42)-C(43)	1.378(5)
C(43)-C(44)	1.384(4)
O(3)-C(46)	1.409(4)
O(3)-C(47)	1.432(4)
C(45)-C(46)	1.441(5)
C(47)-C(48)	1.506(5)

N(6)-Ru(1)-N(2)	171.92(8)
N(6)-Ru(1)-N(4)	91.36(8)
N(2)-Ru(1)-N(4)	94.86(8)
N(6)-Ru(1)-N(5)	78.68(8)
N(2)-Ru(1)-N(5)	95.55(8)
N(4)-Ru(1)-N(5)	95.53(8)
N(6)-Ru(1)-N(3)	98.16(8)
N(2)-Ru(1)-N(3)	88.12(8)
N(4)-Ru(1)-N(3)	78.79(8)
N(5)-Ru(1)-N(3)	173.50(8)
N(6)-Ru(1)-N(1)	95.70(8)
N(2)-Ru(1)-N(1)	78.50(8)
N(4)-Ru(1)-N(1)	171.86(8)
N(5)-Ru(1)-N(1)	89.84(8)
N(3)-Ru(1)-N(1)	96.15(8)
F(1')-P(1)-F(3')	94.5(9)
F(1')-P(1)-F(5)	95.1(9)
F(3')-P(1)-F(5)	132.2(4)
F(1')-P(1)-F(4)	96.4(9)
F(3')-P(1)-F(4)	132.6(5)

F(5)-P(1)-F(4)	92.52(17)
F(1')-P(1)-F(6)	169.0(8)
F(3')-P(1)-F(6)	74.6(4)
F(5)-P(1)-F(6)	91.96(15)
F(4)-P(1)-F(6)	91.65(17)
F(1')-P(1)-F(4')	96.2(10)
F(3')-P(1)-F(4')	92.5(6)
F(5)-P(1)-F(4')	132.6(5)
F(4)-P(1)-F(4')	40.5(5)
F(6)-P(1)-F(4')	85.1(4)
F(1')-P(1)-F(2)	81.9(9)
F(3')-P(1)-F(2)	46.1(4)
F(5)-P(1)-F(2)	89.36(15)
F(4)-P(1)-F(2)	177.58(15)
F(6)-P(1)-F(2)	89.80(16)
F(4')-P(1)-F(2)	137.8(5)
F(1')-P(1)-F(3)	83.3(9)
F(3')-P(1)-F(3)	47.2(4)
F(5)-P(1)-F(3)	178.17(15)
F(4)-P(1)-F(3)	88.65(16)
F(6)-P(1)-F(3)	89.41(15)
F(4')-P(1)-F(3)	48.7(5)
F(2)-P(1)-F(3)	89.43(16)
F(1')-P(1)-F(2')	93.1(10)
F(3')-P(1)-F(2')	92.2(6)
F(5)-P(1)-F(2')	40.6(4)
F(4)-P(1)-F(2')	132.9(4)
F(6)-P(1)-F(2')	86.8(4)
F(4')-P(1)-F(2')	169.2(6)
F(2)-P(1)-F(2')	49.1(4)
F(3)-P(1)-F(2')	138.3(4)
F(1')-P(1)-F(1)	9.8(9)
F(3')-P(1)-F(1)	104.2(4)
F(5)-P(1)-F(1)	89.38(19)
F(4)-P(1)-F(1)	88.72(18)
F(6)-P(1)-F(1)	178.59(19)

F(4')-P(1)-F(1)	94.3(5)
F(2)-P(1)-F(1)	89.78(18)
F(3)-P(1)-F(1)	89.24(19)
F(2')-P(1)-F(1)	94.0(4)
F(1')-P(1)-F(5')	95.7(8)
F(3')-P(1)-F(5')	169.9(6)
F(5)-P(1)-F(5')	46.1(4)
F(4)-P(1)-F(5')	46.5(4)
F(6)-P(1)-F(5')	95.3(4)
F(4')-P(1)-F(5')	87.0(6)
F(2)-P(1)-F(5')	135.2(4)
F(3)-P(1)-F(5')	134.9(4)
F(2')-P(1)-F(5')	86.7(5)
F(1)-P(1)-F(5')	85.9(4)
F(1')-P(1)-F(6')	175.6(10)
F(3')-P(1)-F(6')	89.3(7)
F(5)-P(1)-F(6')	80.7(6)
F(4)-P(1)-F(6')	82.6(7)
F(6)-P(1)-F(6')	14.9(6)
F(4')-P(1)-F(6')	85.8(7)
F(2)-P(1)-F(6')	99.3(6)
F(3)-P(1)-F(6')	100.9(6)
F(2')-P(1)-F(6')	84.5(7)
F(1)-P(1)-F(6')	166.4(6)
F(5')-P(1)-F(6')	80.5(7)
F(8)-P(2)-F(10)	179.58(19)
F(8)-P(2)-F(7)	90.3(2)
F(10)-P(2)-F(7)	89.87(18)
F(8)-P(2)-F(9)	90.2(2)
F(10)-P(2)-F(9)	89.39(18)
F(7)-P(2)-F(9)	92.52(12)
F(8)-P(2)-F(12)	89.3(3)
F(10)-P(2)-F(12)	90.6(2)
F(7)-P(2)-F(12)	178.41(15)
F(9)-P(2)-F(12)	89.02(12)
F(8)-P(2)-F(11)	92.3(2)

F(10)-P(2)-F(11)	88.1(2)
F(7)-P(2)-F(11)	87.69(12)
F(9)-P(2)-F(11)	177.5(2)
F(12)-P(2)-F(11)	90.80(12)
C(1)-N(1)-C(5)	117.69(19)
C(1)-N(1)-Ru(1)	126.03(16)
C(5)-N(1)-Ru(1)	116.28(15)
C(10)-N(2)-C(6)	117.9(2)
C(10)-N(2)-Ru(1)	125.88(16)
C(6)-N(2)-Ru(1)	116.22(15)
C(11)-N(3)-C(15)	117.9(2)
C(11)-N(3)-Ru(1)	126.45(16)
C(15)-N(3)-Ru(1)	115.56(15)
C(20)-N(4)-C(16)	118.3(2)
C(20)-N(4)-Ru(1)	126.05(16)
C(16)-N(4)-Ru(1)	115.53(15)
C(21)-N(5)-C(25)	118.3(2)
C(21)-N(5)-Ru(1)	126.06(18)
C(25)-N(5)-Ru(1)	115.55(16)
C(30)-N(6)-C(26)	118.5(2)
C(30)-N(6)-Ru(1)	125.80(17)
C(26)-N(6)-Ru(1)	115.59(16)
N(1)-C(1)-C(2)	123.7(2)
C(3)-C(2)-C(1)	118.4(2)
O(1)-C(3)-C(2)	122.4(2)
O(1)-C(3)-C(4)	118.3(2)
C(2)-C(3)-C(4)	119.3(2)
C(5)-C(4)-C(3)	119.2(2)
N(1)-C(5)-C(4)	121.8(2)
N(1)-C(5)-C(6)	114.50(19)
C(4)-C(5)-C(6)	123.7(2)
N(2)-C(6)-C(7)	122.0(2)
N(2)-C(6)-C(5)	114.4(2)
C(7)-C(6)-C(5)	123.6(2)
C(6)-C(7)-C(8)	119.0(2)
O(2)-C(8)-C(9)	123.3(2)

O(2)-C(8)-C(7)	117.4(2)
C(9)-C(8)-C(7)	119.3(2)
C(10)-C(9)-C(8)	118.5(2)
N(2)-C(10)-C(9)	123.3(2)
N(3)-C(11)-C(12)	122.9(2)
C(13)-C(12)-C(11)	119.2(2)
C(12)-C(13)-C(14)	118.8(2)
C(15)-C(14)-C(13)	119.7(2)
N(3)-C(15)-C(14)	121.6(2)
N(3)-C(15)-C(16)	114.5(2)
C(14)-C(15)-C(16)	123.8(2)
N(4)-C(16)-C(17)	121.8(2)
N(4)-C(16)-C(15)	115.28(19)
C(17)-C(16)-C(15)	123.0(2)
C(18)-C(17)-C(16)	119.4(2)
C(19)-C(18)-C(17)	119.1(2)
C(18)-C(19)-C(20)	119.0(2)
N(4)-C(20)-C(19)	122.5(2)
N(5)-C(21)-C(22)	122.9(3)
C(21)-C(22)-C(23)	118.5(3)
C(24)-C(23)-C(22)	119.5(3)
C(23)-C(24)-C(25)	119.2(3)
N(5)-C(25)-C(24)	121.4(2)
N(5)-C(25)-C(26)	114.7(2)
C(24)-C(25)-C(26)	123.8(2)
N(6)-C(26)-C(27)	121.0(2)
N(6)-C(26)-C(25)	115.0(2)
C(27)-C(26)-C(25)	123.9(2)
C(28)-C(27)-C(26)	119.9(3)
C(27)-C(28)-C(29)	118.8(3)
C(30)-C(29)-C(28)	119.4(3)
N(6)-C(30)-C(29)	122.4(3)
N(7)-C(31)-C(37)	179.7(6)
C(37)-C(32)-C(33)	118.6(4)
C(34)-C(33)-C(32)	119.1(4)
C(33)-C(34)-C(35)	120.5(4)

C(36)-C(35)-C(34)	121.1(4)
C(35)-C(36)-C(37)	118.5(4)
C(32)-C(37)-C(36)	122.1(4)
C(32)-C(37)-C(31)	118.2(4)
C(36)-C(37)-C(31)	119.6(4)
N(8)-C(38)-C(44)	178.9(4)
C(40)-C(39)-C(44)	119.4(3)
C(39)-C(40)-C(41)	120.2(3)
C(42)-C(41)-C(40)	120.2(3)
C(43)-C(42)-C(41)	120.1(4)
C(42)-C(43)-C(44)	119.3(3)
C(43)-C(44)-C(39)	120.9(3)
C(43)-C(44)-C(38)	119.5(3)
C(39)-C(44)-C(38)	119.6(3)
C(46)-O(3)-C(47)	114.0(3)
O(3)-C(46)-C(45)	112.9(3)
O(3)-C(47)-C(48)	112.7(3)

Symmetry transformations used to generate equivalent atoms:

Table S8. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for paul008. The anisotropic displacement factor exponent takes the form: $-2p^2[h^2 a^{*2}U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ru(1)	16(1)	20(1)	15(1)	1(1)	2(1)	0(1)
P(1)	22(1)	33(1)	18(1)	0(1)	2(1)	1(1)
F(1)	32(2)	42(1)	31(2)	6(1)	-2(1)	10(1)
F(2)	27(1)	44(1)	72(2)	6(1)	9(1)	-7(1)
F(3)	73(2)	64(2)	23(1)	-11(1)	-6(1)	23(1)
F(4)	33(1)	42(1)	94(2)	6(1)	27(1)	-6(1)
F(5)	65(2)	57(2)	24(1)	-15(1)	-4(1)	9(1)
F(6)	48(2)	38(2)	35(2)	6(1)	13(1)	15(1)
F(1')	32(2)	42(1)	31(2)	6(1)	-2(1)	10(1)
F(2')	27(1)	44(1)	72(2)	6(1)	9(1)	-7(1)
F(3')	73(2)	64(2)	23(1)	-11(1)	-6(1)	23(1)
F(4')	33(1)	42(1)	94(2)	6(1)	27(1)	-6(1)
F(5')	65(2)	57(2)	24(1)	-15(1)	-4(1)	9(1)
F(6')	48(2)	38(2)	35(2)	6(1)	13(1)	15(1)
P(2)	34(1)	28(1)	41(1)	11(1)	13(1)	4(1)
F(7)	70(2)	55(1)	62(1)	37(1)	19(1)	9(1)
F(8)	155(3)	77(2)	193(4)	-76(2)	-110(3)	34(2)
F(9)	40(1)	59(1)	90(2)	24(1)	25(1)	10(1)
F(10)	196(4)	110(2)	56(2)	-31(2)	-54(2)	100(3)
F(11)	54(2)	78(2)	186(3)	82(2)	63(2)	38(1)
F(12)	80(2)	86(2)	213(4)	111(2)	96(2)	54(2)
N(1)	18(1)	23(1)	16(1)	1(1)	2(1)	0(1)
N(2)	19(1)	22(1)	18(1)	0(1)	0(1)	-1(1)
N(3)	18(1)	20(1)	20(1)	1(1)	1(1)	0(1)
N(4)	19(1)	23(1)	17(1)	0(1)	1(1)	0(1)
N(5)	19(1)	25(1)	18(1)	4(1)	2(1)	1(1)
N(6)	21(1)	22(1)	17(1)	1(1)	2(1)	0(1)
O(1)	61(2)	53(1)	35(1)	-14(1)	27(1)	-23(1)
O(2)	46(1)	38(1)	35(1)	-8(1)	6(1)	-19(1)
C(1)	25(1)	30(1)	24(1)	-2(1)	6(1)	-6(1)
C(2)	30(1)	33(1)	30(1)	-3(1)	12(1)	-10(1)

C(3)	36(1)	34(1)	24(1)	-2(1)	14(1)	-4(1)
C(4)	33(1)	29(1)	20(1)	-5(1)	8(1)	-4(1)
C(5)	23(1)	21(1)	18(1)	0(1)	3(1)	1(1)
C(6)	20(1)	21(1)	18(1)	0(1)	2(1)	1(1)
C(7)	31(1)	23(1)	20(1)	-2(1)	3(1)	-1(1)
C(8)	29(1)	22(1)	23(1)	-2(1)	-1(1)	-4(1)
C(9)	26(1)	27(1)	25(1)	0(1)	2(1)	-7(1)
C(10)	23(1)	29(1)	18(1)	1(1)	1(1)	-3(1)
C(11)	22(1)	26(1)	24(1)	2(1)	4(1)	2(1)
C(12)	24(1)	28(1)	37(1)	3(1)	2(1)	6(1)
C(13)	28(1)	25(1)	34(1)	5(1)	-2(1)	4(1)
C(14)	28(1)	21(1)	26(1)	5(1)	-1(1)	0(1)
C(15)	21(1)	19(1)	20(1)	0(1)	0(1)	-2(1)
C(16)	22(1)	24(1)	16(1)	1(1)	1(1)	0(1)
C(17)	34(1)	33(1)	21(1)	5(1)	5(1)	2(1)
C(18)	33(1)	44(2)	24(1)	6(1)	10(1)	0(1)
C(19)	26(1)	44(2)	27(1)	1(1)	10(1)	5(1)
C(20)	24(1)	33(1)	22(1)	2(1)	6(1)	5(1)
C(21)	20(1)	34(1)	24(1)	8(1)	-1(1)	-2(1)
C(22)	22(1)	44(2)	36(1)	19(1)	-4(1)	0(1)
C(23)	32(1)	40(2)	49(2)	21(1)	-2(1)	9(1)
C(24)	37(2)	26(1)	44(2)	10(1)	2(1)	6(1)
C(25)	26(1)	24(1)	23(1)	6(1)	2(1)	2(1)
C(26)	27(1)	23(1)	21(1)	0(1)	3(1)	1(1)
C(27)	41(2)	22(1)	33(1)	-2(1)	0(1)	2(1)
C(28)	44(2)	29(1)	32(1)	-8(1)	0(1)	-6(1)
C(29)	30(1)	37(1)	28(1)	-5(1)	-5(1)	-5(1)
C(30)	26(1)	30(1)	23(1)	-3(1)	-2(1)	-1(1)
N(7)	66(2)	53(2)	85(3)	-6(2)	15(2)	7(2)
C(31)	61(2)	56(2)	51(2)	-7(2)	12(2)	-16(2)
C(32)	49(2)	54(2)	63(2)	13(2)	2(2)	-3(2)
C(33)	60(2)	56(2)	52(2)	-1(2)	-4(2)	-15(2)
C(34)	68(2)	35(2)	49(2)	2(2)	1(2)	-8(2)
C(35)	61(2)	51(2)	46(2)	8(2)	0(2)	-1(2)
C(36)	52(2)	54(2)	41(2)	2(2)	4(2)	0(2)
C(37)	42(2)	48(2)	35(2)	6(1)	8(1)	1(1)

N(8)	46(2)	61(2)	58(2)	-22(2)	1(2)	-5(2)
C(38)	38(2)	36(2)	46(2)	-11(1)	7(1)	1(1)
C(39)	38(2)	44(2)	46(2)	-10(1)	16(1)	0(1)
C(40)	29(2)	49(2)	81(3)	-26(2)	16(2)	-3(1)
C(41)	34(2)	65(2)	66(3)	-28(2)	-14(2)	17(2)
C(42)	52(2)	61(2)	46(2)	4(2)	-10(2)	19(2)
C(43)	40(2)	37(2)	46(2)	7(1)	1(1)	6(1)
C(44)	28(1)	31(1)	38(2)	-7(1)	4(1)	5(1)
O(3)	33(1)	33(1)	39(1)	8(1)	4(1)	-5(1)
C(45)	44(2)	73(3)	60(2)	20(2)	0(2)	10(2)
C(46)	45(2)	55(2)	138(5)	52(3)	25(3)	9(2)
C(47)	40(2)	48(2)	49(2)	10(2)	6(1)	7(1)
C(48)	65(3)	58(2)	63(3)	7(2)	20(2)	17(2)

Table S9. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for paul008.

	x	y	z	U(eq)
H(1B)	-1485	1619	7130	58
H(2B)	3901	3565	5476	48
H(1A)	-611	1250	4368	31
H(2A)	-1476	1260	5739	37
H(4A)	623	2330	6553	33
H(7A)	1902	2826	6121	30
H(9A)	3899	3195	4078	31
H(10A)	3115	2579	3226	28
H(11A)	-1012	2304	3608	29
H(12A)	-2056	2889	2845	35
H(13A)	-1403	3209	1499	35
H(14A)	278	2915	942	30
H(17A)	1840	2618	522	35
H(18A)	3524	2250	135	40
H(19A)	4332	1667	1102	39
H(20A)	3448	1468	2421	32
H(21A)	3472	1674	4726	31
H(22A)	4709	1076	5204	41
H(23A)	4433	313	4603	48
H(24A)	2858	162	3617	43
H(27A)	1203	59	2888	38
H(28A)	-566	13	2101	42
H(29A)	-1597	710	1816	38
H(30A)	-844	1428	2309	31
H(32A)	865	430	5441	66
H(33A)	1118	-336	4830	68
H(34A)	2597	-802	5416	61
H(35A)	3856	-511	6528	63
H(36A)	3654	242	7097	59
H(39A)	4949	871	-997	50

H(40A)	6337	1177	17	63
H(41A)	6303	1008	1568	67
H(42A)	4872	538	2106	64
H(43A)	3480	226	1093	49
H(45A)	3561	4784	4012	89
H(45B)	3482	4599	5035	89
H(45C)	3099	4264	4198	89
H(46A)	4936	4247	3761	95
H(46B)	5313	4574	4611	95
H(47A)	6182	3551	5581	54
H(47B)	6560	4068	5280	54
H(48A)	7395	3509	4368	92
H(48B)	6512	3813	3746	92
H(48C)	6182	3293	4068	92

[Ru(bpy)₂(bpy(O)₂)] (paul005a)

Table S10. Crystal data and structure refinement for paul005a.

Identification code	paul005a	
Empirical formula	C ₆₄ H ₆₈ N ₁₄ O ₁₃ Ru ₂	
Formula weight	1443.46	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 23.391(2) Å	a = 90°.
	b = 13.3552(12) Å	b = 99.200(4)°.
	c = 20.5889(19) Å	g = 90°.
Volume	6349.2(10) Å ³	
Z	4	
Density (calculated)	1.510 Mg/m ³	
Absorption coefficient	0.552 mm ⁻¹	
F(000)	2968	
Crystal size	0.13 x 0.10 x 0.10 mm ³	
Theta range for data collection	1.76 to 33.13°.	
Index ranges	-17<=h<=35, -20<=k<=20, -31<=l<=30	
Reflections collected	74556	
Independent reflections	23825 [R(int) = 0.0805]	
Completeness to theta = 25.00°	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9469 and 0.9317	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	23825 / 0 / 894	
Goodness-of-fit on F ²	1.022	
Final R indices [I>2sigma(I)]	R1 = 0.0509, wR2 = 0.1021	
R indices (all data)	R1 = 0.1007, wR2 = 0.1202	
Largest diff. peak and hole	2.656 and -0.931 e.Å ⁻³	

Table S11. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for paul005a. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ru(1)	5830(1)	336(1)	2979(1)	14(1)
Ru(2)	9358(1)	8856(1)	3029(1)	15(1)
N(1)	5509(1)	1478(2)	3495(1)	15(1)
N(2)	6566(1)	782(2)	3605(1)	15(1)
N(3)	5758(1)	-735(2)	3675(1)	18(1)
N(4)	6228(1)	-857(2)	2617(1)	19(1)
N(5)	5922(1)	1363(2)	2264(1)	15(1)
N(6)	5091(1)	76(2)	2313(1)	15(1)
N(7)	8790(1)	8236(2)	3592(1)	17(1)
N(8)	9077(1)	7592(2)	2492(1)	18(1)
N(9)	10084(1)	8097(2)	3465(1)	16(1)
N(10)	9954(1)	9277(2)	2446(1)	16(1)
N(11)	9484(1)	10147(2)	3567(1)	18(1)
N(12)	8672(1)	9701(2)	2584(1)	20(1)
O(1)	4981(1)	3584(1)	4748(1)	21(1)
O(2)	7961(1)	1948(1)	4871(1)	20(1)
O(3)	7537(1)	6919(2)	4524(1)	29(1)
O(4)	8234(1)	5303(2)	1378(1)	57(1)
O(5)	7521(2)	7585(3)	806(1)	71(1)
O(6)	2912(1)	9920(2)	2172(1)	62(1)
O(7)	1686(1)	8692(2)	666(2)	53(1)
O(8)	2685(1)	-22(2)	739(2)	40(1)
O(9)	6907(1)	748(2)	425(1)	33(1)
O(10)	7473(1)	2519(2)	937(1)	33(1)
O(11)	7718(1)	3835(2)	1972(1)	36(1)
O(12)	4204(1)	5120(2)	4569(1)	29(1)
O(13)	1218(1)	9591(2)	4656(1)	29(1)
C(1)	4946(1)	1778(2)	3437(1)	16(1)
C(2)	4756(1)	2479(2)	3834(1)	18(1)
C(3)	5143(1)	2937(2)	4353(1)	17(1)
C(4)	5729(1)	2611(2)	4407(1)	17(1)

C(5)	5892(1)	1915(2)	3980(1)	14(1)
C(6)	6498(1)	1566(2)	4012(1)	15(1)
C(7)	6956(1)	1987(2)	4424(1)	18(1)
C(8)	7527(1)	1592(2)	4468(1)	16(1)
C(9)	7579(1)	764(2)	4051(1)	17(1)
C(10)	7106(1)	410(2)	3640(1)	18(1)
C(11)	5491(1)	-624(2)	4208(1)	22(1)
C(12)	5569(2)	-1280(2)	4727(2)	30(1)
C(13)	5940(1)	-2082(2)	4720(2)	33(1)
C(14)	6205(1)	-2227(2)	4176(2)	30(1)
C(15)	6100(1)	-1552(2)	3651(1)	22(1)
C(16)	6342(1)	-1642(2)	3038(1)	22(1)
C(17)	6660(1)	-2471(2)	2884(2)	32(1)
C(18)	6858(1)	-2492(3)	2293(2)	37(1)
C(19)	6726(1)	-1711(3)	1853(2)	33(1)
C(20)	6413(1)	-901(2)	2029(1)	23(1)
C(21)	6348(1)	2048(2)	2293(1)	19(1)
C(22)	6363(1)	2763(2)	1815(1)	22(1)
C(23)	5923(1)	2778(2)	1274(1)	25(1)
C(24)	5484(1)	2083(2)	1238(1)	24(1)
C(25)	5490(1)	1389(2)	1738(1)	17(1)
C(26)	5032(1)	635(2)	1754(1)	18(1)
C(27)	4574(1)	491(2)	1246(1)	22(1)
C(28)	4155(1)	-207(2)	1313(1)	24(1)
C(29)	4207(1)	-760(2)	1888(1)	22(1)
C(30)	4681(1)	-606(2)	2372(1)	20(1)
C(31)	8654(1)	8608(2)	4162(1)	19(1)
C(32)	8242(1)	8200(2)	4485(1)	23(1)
C(33)	7932(1)	7334(2)	4239(1)	22(1)
C(34)	8089(1)	6948(2)	3648(1)	20(1)
C(35)	8498(1)	7406(2)	3342(1)	17(1)
C(36)	8648(1)	7056(2)	2708(1)	17(1)
C(37)	8368(1)	6281(2)	2350(1)	24(1)
C(38)	8501(1)	6005(2)	1731(2)	30(1)
C(39)	8947(1)	6569(2)	1518(1)	26(1)
C(40)	9217(1)	7318(2)	1903(1)	23(1)

C(41)	10121(1)	7499(2)	3994(1)	20(1)
C(42)	10618(1)	6971(2)	4242(1)	21(1)
C(43)	11101(1)	7065(2)	3940(1)	21(1)
C(44)	11071(1)	7684(2)	3398(1)	21(1)
C(45)	10562(1)	8186(2)	3170(1)	17(1)
C(46)	10482(1)	8844(2)	2590(1)	16(1)
C(47)	10909(1)	9001(2)	2199(1)	23(1)
C(48)	10790(1)	9595(2)	1644(1)	25(1)
C(49)	10253(1)	10046(2)	1505(1)	24(1)
C(50)	9855(1)	9891(2)	1916(1)	21(1)
C(51)	9917(1)	10334(2)	4066(1)	22(1)
C(52)	9961(2)	11220(2)	4419(2)	30(1)
C(53)	9547(2)	11952(2)	4254(2)	38(1)
C(54)	9092(2)	11769(2)	3747(2)	34(1)
C(55)	9068(1)	10867(2)	3411(1)	22(1)
C(56)	8610(1)	10610(2)	2860(1)	23(1)
C(57)	8146(1)	11235(3)	2627(2)	33(1)
C(58)	7751(1)	10939(3)	2091(2)	40(1)
C(59)	7819(1)	10020(3)	1800(2)	34(1)
C(60)	8279(1)	9422(2)	2067(1)	27(1)
N(13)	9556(2)	8813(3)	31(2)	55(1)
C(61)	8621(2)	9360(3)	435(2)	44(1)
C(62)	9143(2)	9039(2)	204(2)	32(1)
N(14)	3667(2)	368(2)	3546(2)	51(1)
C(63)	3066(2)	134(4)	4484(2)	64(1)
C(64)	3404(2)	279(3)	3961(2)	42(1)

Table S12. Bond lengths [Å] and angles [°] for paul005a.

Ru(1)-N(4)	2.044(2)
Ru(1)-N(5)	2.048(2)
Ru(1)-N(3)	2.051(2)
Ru(1)-N(6)	2.057(2)
Ru(1)-N(2)	2.066(2)
Ru(1)-N(1)	2.068(2)
Ru(2)-N(11)	2.044(2)
Ru(2)-N(12)	2.054(2)
Ru(2)-N(9)	2.056(2)
Ru(2)-N(10)	2.058(2)
Ru(2)-N(8)	2.068(2)
Ru(2)-N(7)	2.072(2)
N(1)-C(5)	1.363(3)
N(1)-C(1)	1.363(3)
N(2)-C(10)	1.350(3)
N(2)-C(6)	1.365(3)
N(3)-C(11)	1.354(4)
N(3)-C(15)	1.357(4)
N(4)-C(20)	1.350(4)
N(4)-C(16)	1.360(4)
N(5)-C(21)	1.346(3)
N(5)-C(25)	1.358(3)
N(6)-C(30)	1.343(3)
N(6)-C(26)	1.360(3)
N(7)-C(31)	1.356(3)
N(7)-C(35)	1.359(3)
N(8)-C(40)	1.354(3)
N(8)-C(36)	1.363(3)
N(9)-C(41)	1.344(3)
N(9)-C(45)	1.361(3)
N(10)-C(46)	1.354(3)
N(10)-C(50)	1.355(3)
N(11)-C(51)	1.344(3)
N(11)-C(55)	1.370(3)

N(12)-C(60)	1.343(4)
N(12)-C(56)	1.359(4)
O(1)-C(3)	1.283(3)
O(2)-C(8)	1.294(3)
O(3)-C(33)	1.296(3)
O(4)-C(38)	1.284(4)
C(1)-C(2)	1.364(4)
C(2)-C(3)	1.423(4)
C(3)-C(4)	1.427(4)
C(4)-C(5)	1.373(3)
C(5)-C(6)	1.483(4)
C(6)-C(7)	1.377(3)
C(7)-C(8)	1.425(4)
C(8)-C(9)	1.416(4)
C(9)-C(10)	1.366(4)
C(11)-C(12)	1.372(4)
C(12)-C(13)	1.379(5)
C(13)-C(14)	1.378(5)
C(14)-C(15)	1.399(4)
C(15)-C(16)	1.471(4)
C(16)-C(17)	1.398(4)
C(17)-C(18)	1.370(5)
C(18)-C(19)	1.383(5)
C(19)-C(20)	1.387(4)
C(21)-C(22)	1.375(4)
C(22)-C(23)	1.390(4)
C(23)-C(24)	1.378(4)
C(24)-C(25)	1.385(4)
C(25)-C(26)	1.474(4)
C(26)-C(27)	1.386(4)
C(27)-C(28)	1.376(4)
C(28)-C(29)	1.384(4)
C(29)-C(30)	1.382(4)
C(31)-C(32)	1.370(4)
C(32)-C(33)	1.414(4)
C(33)-C(34)	1.422(4)

C(34)-C(35)	1.370(4)
C(35)-C(36)	1.482(4)
C(36)-C(37)	1.374(4)
C(37)-C(38)	1.410(4)
C(38)-C(39)	1.413(4)
C(39)-C(40)	1.367(4)
C(41)-C(42)	1.385(4)
C(42)-C(43)	1.381(4)
C(43)-C(44)	1.380(4)
C(44)-C(45)	1.382(4)
C(45)-C(46)	1.471(4)
C(46)-C(47)	1.394(4)
C(47)-C(48)	1.383(4)
C(48)-C(49)	1.382(4)
C(49)-C(50)	1.371(4)
C(51)-C(52)	1.385(4)
C(52)-C(53)	1.379(5)
C(53)-C(54)	1.389(5)
C(54)-C(55)	1.387(4)
C(55)-C(56)	1.470(4)
C(56)-C(57)	1.392(4)
C(57)-C(58)	1.379(5)
C(58)-C(59)	1.386(5)
C(59)-C(60)	1.382(4)
N(13)-C(62)	1.122(4)
C(61)-C(62)	1.445(5)
N(14)-C(64)	1.137(5)
C(63)-C(64)	1.447(6)
N(4)-Ru(1)-N(5)	98.82(9)
N(4)-Ru(1)-N(3)	78.77(9)
N(5)-Ru(1)-N(3)	177.58(9)
N(4)-Ru(1)-N(6)	90.51(9)
N(5)-Ru(1)-N(6)	78.90(8)
N(3)-Ru(1)-N(6)	101.19(9)
N(4)-Ru(1)-N(2)	94.05(8)

N(5)-Ru(1)-N(2)	94.75(8)
N(3)-Ru(1)-N(2)	85.31(9)
N(6)-Ru(1)-N(2)	172.70(9)
N(4)-Ru(1)-N(1)	170.42(8)
N(5)-Ru(1)-N(1)	87.92(8)
N(3)-Ru(1)-N(1)	94.47(9)
N(6)-Ru(1)-N(1)	97.51(8)
N(2)-Ru(1)-N(1)	78.52(8)
N(11)-Ru(2)-N(12)	79.25(9)
N(11)-Ru(2)-N(9)	98.14(9)
N(12)-Ru(2)-N(9)	175.83(9)
N(11)-Ru(2)-N(10)	91.91(9)
N(12)-Ru(2)-N(10)	98.27(9)
N(9)-Ru(2)-N(10)	78.50(9)
N(11)-Ru(2)-N(8)	169.86(9)
N(12)-Ru(2)-N(8)	92.93(9)
N(9)-Ru(2)-N(8)	90.02(9)
N(10)-Ru(2)-N(8)	95.62(9)
N(11)-Ru(2)-N(7)	94.80(9)
N(12)-Ru(2)-N(7)	86.73(9)
N(9)-Ru(2)-N(7)	96.76(8)
N(10)-Ru(2)-N(7)	172.29(9)
N(8)-Ru(2)-N(7)	78.19(9)
C(5)-N(1)-C(1)	116.8(2)
C(5)-N(1)-Ru(1)	116.24(17)
C(1)-N(1)-Ru(1)	126.66(17)
C(10)-N(2)-C(6)	116.7(2)
C(10)-N(2)-Ru(1)	127.30(17)
C(6)-N(2)-Ru(1)	115.97(16)
C(11)-N(3)-C(15)	117.9(2)
C(11)-N(3)-Ru(1)	126.15(19)
C(15)-N(3)-Ru(1)	114.82(19)
C(20)-N(4)-C(16)	118.6(2)
C(20)-N(4)-Ru(1)	126.2(2)
C(16)-N(4)-Ru(1)	115.01(18)
C(21)-N(5)-C(25)	117.9(2)

C(21)-N(5)-Ru(1)	125.82(17)
C(25)-N(5)-Ru(1)	116.08(17)
C(30)-N(6)-C(26)	118.1(2)
C(30)-N(6)-Ru(1)	126.23(18)
C(26)-N(6)-Ru(1)	115.60(17)
C(31)-N(7)-C(35)	117.0(2)
C(31)-N(7)-Ru(2)	126.66(18)
C(35)-N(7)-Ru(2)	116.24(17)
C(40)-N(8)-C(36)	116.5(2)
C(40)-N(8)-Ru(2)	126.67(19)
C(36)-N(8)-Ru(2)	116.22(18)
C(41)-N(9)-C(45)	117.5(2)
C(41)-N(9)-Ru(2)	126.11(19)
C(45)-N(9)-Ru(2)	116.34(16)
C(46)-N(10)-C(50)	117.9(2)
C(46)-N(10)-Ru(2)	115.74(17)
C(50)-N(10)-Ru(2)	126.20(19)
C(51)-N(11)-C(55)	117.9(2)
C(51)-N(11)-Ru(2)	126.61(19)
C(55)-N(11)-Ru(2)	115.40(18)
C(60)-N(12)-C(56)	118.3(2)
C(60)-N(12)-Ru(2)	126.0(2)
C(56)-N(12)-Ru(2)	115.65(18)
N(1)-C(1)-C(2)	123.5(2)
C(1)-C(2)-C(3)	121.1(2)
O(1)-C(3)-C(2)	123.2(2)
O(1)-C(3)-C(4)	122.3(2)
C(2)-C(3)-C(4)	114.5(2)
C(5)-C(4)-C(3)	121.3(2)
N(1)-C(5)-C(4)	122.8(2)
N(1)-C(5)-C(6)	114.2(2)
C(4)-C(5)-C(6)	123.1(2)
N(2)-C(6)-C(7)	122.4(2)
N(2)-C(6)-C(5)	114.7(2)
C(7)-C(6)-C(5)	122.9(2)
C(6)-C(7)-C(8)	121.1(2)

O(2)-C(8)-C(9)	122.7(2)
O(2)-C(8)-C(7)	122.3(2)
C(9)-C(8)-C(7)	114.9(2)
C(10)-C(9)-C(8)	120.4(2)
N(2)-C(10)-C(9)	124.4(2)
N(3)-C(11)-C(12)	122.6(3)
C(11)-C(12)-C(13)	119.6(3)
C(14)-C(13)-C(12)	118.9(3)
C(13)-C(14)-C(15)	119.4(3)
N(3)-C(15)-C(14)	121.5(3)
N(3)-C(15)-C(16)	114.1(2)
C(14)-C(15)-C(16)	124.5(3)
N(4)-C(16)-C(17)	121.6(3)
N(4)-C(16)-C(15)	114.9(2)
C(17)-C(16)-C(15)	123.5(3)
C(18)-C(17)-C(16)	119.0(3)
C(17)-C(18)-C(19)	119.7(3)
C(18)-C(19)-C(20)	119.2(3)
N(4)-C(20)-C(19)	121.8(3)
N(5)-C(21)-C(22)	123.0(2)
C(21)-C(22)-C(23)	118.8(3)
C(24)-C(23)-C(22)	118.9(3)
C(23)-C(24)-C(25)	119.4(3)
N(5)-C(25)-C(24)	121.9(2)
N(5)-C(25)-C(26)	114.6(2)
C(24)-C(25)-C(26)	123.5(2)
N(6)-C(26)-C(27)	121.6(2)
N(6)-C(26)-C(25)	114.7(2)
C(27)-C(26)-C(25)	123.7(2)
C(28)-C(27)-C(26)	119.7(3)
C(27)-C(28)-C(29)	118.7(3)
C(30)-C(29)-C(28)	119.2(3)
N(6)-C(30)-C(29)	122.6(3)
N(7)-C(31)-C(32)	123.7(3)
C(31)-C(32)-C(33)	120.7(3)
O(3)-C(33)-C(32)	123.3(3)

O(3)-C(33)-C(34)	122.1(3)
C(32)-C(33)-C(34)	114.7(3)
C(35)-C(34)-C(33)	121.6(3)
N(7)-C(35)-C(34)	122.4(3)
N(7)-C(35)-C(36)	114.5(2)
C(34)-C(35)-C(36)	123.1(2)
N(8)-C(36)-C(37)	122.3(3)
N(8)-C(36)-C(35)	114.4(2)
C(37)-C(36)-C(35)	123.3(2)
C(36)-C(37)-C(38)	121.7(3)
O(4)-C(38)-C(37)	123.1(3)
O(4)-C(38)-C(39)	122.0(3)
C(37)-C(38)-C(39)	114.9(3)
C(40)-C(39)-C(38)	120.5(3)
N(8)-C(40)-C(39)	124.1(3)
N(9)-C(41)-C(42)	122.9(3)
C(43)-C(42)-C(41)	119.1(3)
C(44)-C(43)-C(42)	118.6(3)
C(43)-C(44)-C(45)	119.6(3)
N(9)-C(45)-C(44)	122.2(2)
N(9)-C(45)-C(46)	114.0(2)
C(44)-C(45)-C(46)	123.9(2)
N(10)-C(46)-C(47)	121.4(2)
N(10)-C(46)-C(45)	115.3(2)
C(47)-C(46)-C(45)	123.3(2)
C(48)-C(47)-C(46)	119.8(3)
C(49)-C(48)-C(47)	118.5(3)
C(50)-C(49)-C(48)	119.4(3)
N(10)-C(50)-C(49)	122.9(3)
N(11)-C(51)-C(52)	123.0(3)
C(53)-C(52)-C(51)	119.0(3)
C(52)-C(53)-C(54)	119.0(3)
C(55)-C(54)-C(53)	119.5(3)
N(11)-C(55)-C(54)	121.5(3)
N(11)-C(55)-C(56)	114.9(2)
C(54)-C(55)-C(56)	123.6(3)

N(12)-C(56)-C(57)	121.4(3)
N(12)-C(56)-C(55)	114.6(2)
C(57)-C(56)-C(55)	124.0(3)
C(58)-C(57)-C(56)	119.3(3)
C(57)-C(58)-C(59)	119.5(3)
C(60)-C(59)-C(58)	118.4(3)
N(12)-C(60)-C(59)	123.1(3)
N(13)-C(62)-C(61)	178.2(4)
N(14)-C(64)-C(63)	178.3(4)

Symmetry transformations used to generate equivalent atoms:

Table S13. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for paul005a. The anisotropic displacement factor exponent takes the form: $-2p^2 [h^2 a^* U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ru(1)	13(1)	15(1)	13(1)	-3(1)	2(1)	-1(1)
Ru(2)	13(1)	15(1)	16(1)	1(1)	3(1)	1(1)
N(1)	14(1)	15(1)	14(1)	-2(1)	2(1)	0(1)
N(2)	13(1)	16(1)	17(1)	-3(1)	2(1)	1(1)
N(3)	17(1)	17(1)	19(1)	-1(1)	0(1)	-2(1)
N(4)	17(1)	19(1)	20(1)	-8(1)	1(1)	-2(1)
N(5)	16(1)	17(1)	13(1)	-3(1)	3(1)	-1(1)
N(6)	14(1)	16(1)	14(1)	-4(1)	2(1)	-2(1)
N(7)	15(1)	18(1)	18(1)	2(1)	4(1)	2(1)
N(8)	16(1)	20(1)	18(1)	-1(1)	4(1)	-2(1)
N(9)	17(1)	15(1)	16(1)	1(1)	3(1)	0(1)
N(10)	16(1)	15(1)	18(1)	-1(1)	2(1)	-2(1)
N(11)	20(1)	17(1)	20(1)	0(1)	8(1)	-1(1)
N(12)	16(1)	23(1)	21(1)	7(1)	6(1)	1(1)
O(1)	22(1)	19(1)	22(1)	-6(1)	3(1)	6(1)
O(2)	14(1)	24(1)	20(1)	-2(1)	-2(1)	-1(1)
O(3)	25(1)	31(1)	35(1)	7(1)	16(1)	-3(1)
O(4)	60(2)	70(2)	45(2)	-34(1)	25(1)	-45(2)
O(5)	89(2)	86(2)	48(2)	14(2)	40(2)	42(2)
O(6)	49(2)	87(2)	48(2)	-9(2)	2(1)	29(2)
O(7)	53(2)	39(2)	75(2)	-17(2)	31(2)	3(2)
O(8)	33(1)	38(2)	49(2)	-13(1)	1(1)	7(1)
O(9)	25(1)	38(1)	36(1)	-5(1)	2(1)	-6(1)
O(10)	37(1)	40(2)	24(1)	3(1)	5(1)	-16(1)
O(11)	26(1)	44(2)	38(1)	-10(1)	7(1)	-9(1)
O(12)	24(1)	24(1)	37(1)	-5(1)	-2(1)	7(1)
O(13)	29(1)	28(1)	29(1)	2(1)	4(1)	9(1)
C(1)	13(1)	20(1)	15(1)	0(1)	0(1)	1(1)
C(2)	15(1)	20(1)	19(1)	0(1)	1(1)	3(1)
C(3)	18(1)	16(1)	18(1)	2(1)	3(1)	3(1)
C(4)	16(1)	16(1)	18(1)	-2(1)	-1(1)	4(1)

C(5)	15(1)	13(1)	13(1)	0(1)	2(1)	-1(1)
C(6)	16(1)	15(1)	14(1)	1(1)	0(1)	1(1)
C(7)	16(1)	17(1)	19(1)	-2(1)	0(1)	1(1)
C(8)	18(1)	18(1)	14(1)	1(1)	3(1)	-2(1)
C(9)	13(1)	20(1)	20(1)	0(1)	4(1)	3(1)
C(10)	17(1)	19(1)	18(1)	-4(1)	4(1)	2(1)
C(11)	26(2)	22(1)	19(1)	0(1)	4(1)	-3(1)
C(12)	38(2)	30(2)	23(1)	4(1)	6(1)	-5(2)
C(13)	32(2)	33(2)	32(2)	12(1)	1(1)	-3(2)
C(14)	26(2)	21(2)	42(2)	7(1)	-1(1)	1(1)
C(15)	19(1)	18(1)	26(1)	-2(1)	-2(1)	-3(1)
C(16)	16(1)	18(1)	32(2)	-7(1)	1(1)	-2(1)
C(17)	27(2)	25(2)	44(2)	-9(1)	4(1)	2(1)
C(18)	22(2)	28(2)	60(2)	-18(2)	6(2)	4(1)
C(19)	20(2)	41(2)	39(2)	-22(2)	10(1)	-6(1)
C(20)	18(1)	26(2)	26(1)	-13(1)	6(1)	-4(1)
C(21)	14(1)	23(1)	20(1)	-1(1)	3(1)	-3(1)
C(22)	19(1)	21(1)	27(1)	-4(1)	6(1)	-5(1)
C(23)	30(2)	25(2)	22(1)	4(1)	4(1)	-4(1)
C(24)	25(2)	24(1)	22(1)	1(1)	0(1)	-8(1)
C(25)	17(1)	17(1)	17(1)	-2(1)	4(1)	-1(1)
C(26)	21(1)	18(1)	16(1)	-3(1)	4(1)	-2(1)
C(27)	22(1)	24(2)	20(1)	1(1)	-1(1)	-3(1)
C(28)	20(1)	28(2)	24(1)	-6(1)	-3(1)	-3(1)
C(29)	17(1)	22(1)	28(1)	-3(1)	2(1)	-7(1)
C(30)	20(1)	20(1)	20(1)	-1(1)	4(1)	-4(1)
C(31)	19(1)	19(1)	20(1)	2(1)	5(1)	3(1)
C(32)	25(1)	24(2)	21(1)	3(1)	9(1)	6(1)
C(33)	19(1)	22(1)	24(1)	8(1)	6(1)	5(1)
C(34)	21(1)	18(1)	24(1)	3(1)	5(1)	1(1)
C(35)	15(1)	16(1)	20(1)	4(1)	2(1)	1(1)
C(36)	13(1)	18(1)	21(1)	1(1)	3(1)	1(1)
C(37)	23(1)	24(2)	26(1)	-5(1)	6(1)	-5(1)
C(38)	29(2)	33(2)	28(2)	-10(1)	7(1)	-10(1)
C(39)	27(2)	29(2)	22(1)	-8(1)	7(1)	-5(1)
C(40)	20(1)	26(2)	24(1)	-4(1)	7(1)	-3(1)

C(41)	20(1)	20(1)	19(1)	1(1)	4(1)	0(1)
C(42)	23(1)	21(1)	19(1)	2(1)	1(1)	4(1)
C(43)	17(1)	20(1)	24(1)	0(1)	-2(1)	5(1)
C(44)	14(1)	24(1)	26(1)	0(1)	4(1)	1(1)
C(45)	16(1)	16(1)	19(1)	0(1)	4(1)	1(1)
C(46)	15(1)	16(1)	17(1)	-2(1)	2(1)	0(1)
C(47)	18(1)	24(2)	28(1)	3(1)	8(1)	2(1)
C(48)	26(2)	29(2)	23(1)	1(1)	11(1)	-4(1)
C(49)	29(2)	24(1)	20(1)	4(1)	6(1)	-2(1)
C(50)	21(1)	21(1)	22(1)	4(1)	3(1)	2(1)
C(51)	23(1)	23(1)	20(1)	0(1)	7(1)	-4(1)
C(52)	39(2)	27(2)	25(1)	-4(1)	9(1)	-7(2)
C(53)	67(3)	21(2)	30(2)	-8(1)	19(2)	-1(2)
C(54)	53(2)	21(2)	32(2)	3(1)	20(2)	10(2)
C(55)	28(2)	18(1)	23(1)	4(1)	13(1)	4(1)
C(56)	23(1)	25(2)	24(1)	10(1)	13(1)	9(1)
C(57)	34(2)	35(2)	35(2)	20(1)	19(1)	18(2)
C(58)	25(2)	56(2)	42(2)	30(2)	14(2)	20(2)
C(59)	16(1)	54(2)	30(2)	19(2)	1(1)	1(2)
C(60)	18(1)	37(2)	25(1)	9(1)	2(1)	-2(1)
N(13)	54(2)	64(2)	49(2)	-21(2)	17(2)	2(2)
C(61)	35(2)	58(2)	40(2)	-15(2)	8(2)	4(2)
C(62)	42(2)	30(2)	23(2)	-4(1)	5(1)	-3(2)
N(14)	63(2)	34(2)	58(2)	-3(2)	13(2)	-4(2)
C(63)	71(3)	81(3)	39(2)	8(2)	3(2)	-38(3)
C(64)	56(2)	27(2)	42(2)	5(2)	0(2)	-14(2)

Table S14. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for paul005a.

	x	y	z	U(eq)
H(7C)	1815(17)	8170(30)	490(19)	47(9)
H(7B)	1975(18)	8890(30)	760(20)	47(9)
H(8B)	2810(20)	-30(40)	1080(30)	75(19)
H(8C)	2683(16)	600(30)	661(18)	37(11)
H(9B)	6590(20)	480(30)	380(20)	72(16)
H(9C)	7003(19)	500(30)	170(20)	42(14)
H(10B)	7263(18)	2030(30)	810(20)	53(13)
H(10C)	7619(19)	2650(30)	650(20)	56(15)
H(11B)	7842(16)	4220(30)	1789(18)	29(7)
H(11C)	7593(15)	3420(30)	1666(17)	29(7)
H(12B)	4446(18)	5520(30)	4750(20)	47(12)
H(12C)	4379(16)	4640(30)	4602(18)	35(11)
H(13B)	1396(14)	9760(30)	4387(17)	24(10)
H(13C)	1420(17)	9090(30)	4840(20)	48(12)
H(1)	4672	1484	3101	20
H(2)	4359	2664	3764	22
H(4)	6012	2880	4744	21
H(7)	6891	2550	4684	21
H(9)	7945	453	4058	21
H(10)	7162	-133	3359	21
H(11)	5238	-70	4222	27
H(12)	5370	-1182	5090	36
H(13)	6011	-2527	5084	39
H(14)	6457	-2780	4158	36
H(17)	6738	-3011	3186	39
H(18)	7084	-3040	2186	44
H(19)	6849	-1730	1435	39
H(20)	6327	-363	1728	28
H(21A)	6651	2036	2659	23
H(22A)	6669	3238	1854	27

H(23A)	5926	3261	936	31
H(24A)	5180	2081	872	29
H(27A)	4550	872	853	27
H(28A)	3836	-307	972	29
H(29A)	3921	-1239	1949	27
H(30A)	4718	-999	2761	24
H(31A)	8857	9183	4347	23
H(32A)	8162	8502	4879	27
H(34A)	7905	6357	3460	25
H(37A)	8076	5923	2525	29
H(39A)	9060	6428	1105	31
H(40A)	9522	7669	1749	28
H(41A)	9792	7435	4209	23
H(42A)	10625	6549	4615	25
H(43A)	11447	6712	4102	25
H(44A)	11399	7763	3184	25
H(47A)	11279	8701	2314	27
H(48A)	11072	9692	1365	30
H(49A)	10160	10459	1127	29
H(50A)	9493	10229	1825	25
H(51A)	10205	9836	4180	26
H(52A)	10272	11323	4770	36
H(53A)	9573	12571	4484	46
H(54A)	8799	12259	3632	41
H(57A)	8102	11860	2835	40
H(58A)	7435	11361	1923	48
H(59A)	7555	9806	1426	40
H(60A)	8320	8784	1876	33
H(61A)	8720	9645	877	66
H(61B)	8363	8785	448	66
H(61C)	8425	9869	135	66
H(63A)	2654	115	4298	96
H(63B)	3139	688	4798	96
H(63C)	3177	-500	4709	96

Computational Information

The cartesian coordinates (in Å) of the symmetry unique atoms in the gas-phase optimized structures reported in this manuscript are given below. The nuclear repulsion and total energies are also reported, along with the point group used to run the calculation.

Nuclear Repulsion Energy (a.u.) = 4288.0506923

Total Energy (a.u.) = -1555.1309286

C₂ symmetry

RU	44.0	0.0000000000	0.0000000000	0.1891471133
N	7.0	1.1282248121	0.6986286975	-1.4456483340
N	7.0	1.2654300902	-1.6758238911	0.3343080030
N	7.0	1.3608206966	0.6053332510	1.6789756583
H	1.0	2.9010198184	1.9659255752	-4.6563829475
C	6.0	0.6197738063	0.4018756319	-2.6757062941
C	6.0	1.2475189106	0.8500236876	-3.8431056432
H	1.0	0.8304971815	0.6175105656	-4.8155100292
C	6.0	2.4113515540	1.6093377590	-3.7554192334
C	6.0	2.9308656973	1.8998435335	-2.4942498828
H	1.0	3.8333123964	2.4897527045	-2.3755096996
C	6.0	2.2608038430	1.4243561099	-1.3712441481
H	1.0	2.6255036522	1.6343906815	-0.3728669108
C	6.0	1.1457719463	-2.8150419263	-0.3749120633
H	1.0	0.3340995108	-2.8456698346	-1.0919785714
C	6.0	1.9998361984	-3.9015203914	-0.2105743972
H	1.0	1.8547948503	-4.7968301328	-0.8058673085
C	6.0	3.0275591220	-3.8094972341	0.7276280457
H	1.0	3.7124780136	-4.6361999638	0.8888847897
C	6.0	3.1639562655	-2.6329665884	1.4592439057
H	1.0	3.9529598028	-2.5470646234	2.1965623512
C	6.0	2.2718097774	-1.5759078766	1.2486750186
C	6.0	2.3336155252	-0.2987664146	1.9875876509
C	6.0	3.3194991360	-0.0034699589	2.9353675394
H	1.0	4.0948875207	-0.7241671684	3.1658306629
C	6.0	3.3104538522	1.2295624605	3.5819412504
H	1.0	4.0760829905	1.4686872092	4.3133132510
C	6.0	2.3075949808	2.1458339140	3.2658686933
H	1.0	2.2567215648	3.1172404495	3.7459535039
C	6.0	1.3549529083	1.7930523014	2.3144798782
H	1.0	0.5593187540	2.4763443342	2.0423756928

Nuclear Repulsion Energy (a.u.) = 4676.6780546

Total Energy (a.u.) = -1705.5095797

C₂ symmetry

RU	44.0	0.0000000000	0.0000000000	0.2091495623
N	7.0	1.1233831262	0.6984092527	-1.4329288143
N	7.0	1.2561174267	-1.6767748368	0.3489580918
N	7.0	1.3638860701	0.6042439333	1.6867679178
O	8.0	3.0274980010	2.1647114675	-4.8050266634
H	1.0	2.5958328071	1.9278138172	-5.6428677486
C	6.0	0.6170176979	0.4102756157	-2.6636754161
C	6.0	1.2206184808	0.8802882332	-3.8304268524
H	1.0	0.7913963324	0.6605423333	-4.8019259763
C	6.0	2.3823662152	1.6601720243	-3.7465628228
C	6.0	2.9087955828	1.9359395237	-2.4743987474
H	1.0	3.8102360684	2.5302149219	-2.3761739880
C	6.0	2.2530056708	1.4358713108	-1.3653457163
H	1.0	2.6282168391	1.6384071065	-0.3690858403
C	6.0	1.1267321271	-2.8162351266	-0.3578566900
H	1.0	0.3093383220	-2.8443567141	-1.0690180896
C	6.0	1.9734036271	-3.9081380378	-0.1923922661
H	1.0	1.8171082220	-4.8060254452	-0.7808096683
C	6.0	3.0044545982	-3.8203981129	0.7430795764
H	1.0	3.6805050849	-4.6536286069	0.9084728981
C	6.0	3.1511292862	-2.6426964840	1.4710637475
H	1.0	3.9440772298	-2.5581600424	2.2044095140
C	6.0	2.2690084802	-1.5783133503	1.2560696985
C	6.0	2.3432941101	-0.2964231838	1.9849444380
C	6.0	3.3452093083	0.0083896333	2.9124454153
H	1.0	4.1272269954	-0.7088598563	3.1314061833
C	6.0	3.3446635856	1.2459978077	3.5503761523
H	1.0	4.1227763315	1.4928139877	4.2661248101
C	6.0	2.3307833515	2.1557026696	3.2496750321
H	1.0	2.2865617028	3.1310081185	3.7226708844
C	6.0	1.3628852861	1.7947859756	2.3172775588
H	1.0	0.5615935416	2.4751452896	2.0526786000

Nuclear Repulsion Energy (a.u.) = 4654.9214456

Total Energy (a.u.) = -1705.1502743

C₁ symmetry

RU	44.0	0.0688625143	0.0325743211	0.0581723102
N	7.0	-0.9658148252	-0.7955242046	-1.5709201980
N	7.0	1.0811490583	0.8677262642	-1.5571622701
N	7.0	1.4886754488	-1.4862330706	0.2415612977
N	7.0	1.3274874417	0.8041578095	1.5418820348
N	7.0	-1.3345452114	1.5679080949	0.2252045477
N	7.0	-1.2389445417	-0.7305879405	1.5265455092
O	8.0	2.9347042358	2.2495185379	-4.9965527294
C	6.0	-2.0356408612	-1.6105815761	-1.4947954882
H	1.0	-2.3670989876	-1.8691527857	-0.4957573270
C	6.0	-2.6949488610	-2.1158102018	-2.6013241300
H	1.0	-3.5516167155	-2.7718338791	-2.4738906789
C	6.0	-2.2264199424	-1.7514470700	-3.8734830156
C	6.0	-1.1214314984	-0.9031024533	-3.9651670568
H	1.0	-0.7625919211	-0.6156545120	-4.9450502843
C	6.0	-0.5055921711	-0.4286032270	-2.8064281067
C	6.0	0.6528980644	0.4858797883	-2.8109562162
C	6.0	1.2501694143	0.9277526429	-3.9686016165
H	1.0	0.8973723878	0.6102651028	-4.9439628815
C	6.0	2.3888646123	1.8447898284	-3.9619953549
C	6.0	2.7867037120	2.2223381826	-2.6115475809
H	1.0	3.6236235938	2.9039855202	-2.4932378323
C	6.0	2.1404449222	1.7275779470	-1.5111256885
H	1.0	2.4616290074	2.0121933773	-0.5131160571
C	6.0	1.5422053134	-2.6141459009	-0.4939369083
H	1.0	0.8229093388	-2.6806594357	-1.3008261790
C	6.0	2.4520314876	-3.6365230261	-0.2469744735
H	1.0	2.4497472344	-4.5222105747	-0.8735880400
C	6.0	3.3496298913	-3.4956912290	0.8115342069
H	1.0	4.0667637954	-4.2769769571	1.0433560110
C	6.0	3.3209267606	-2.3227931228	1.5600148368
H	1.0	4.0181705607	-2.1891822111	2.3789320105
C	6.0	2.3938441968	-1.3221818109	1.2500045296
C	6.0	2.3244199212	-0.0286464381	1.9541995680
C	6.0	3.2310467072	0.3661866371	2.9445657241
H	1.0	4.0182291370	-0.3056156506	3.2658158932
C	6.0	3.1377002148	1.6376432446	3.5017980198
H	1.0	3.8402048867	1.9555380031	4.2657493166

C	6.0	2.1307477526	2.4934509548	3.0547257889
H	1.0	2.0263336143	3.5004260120	3.4447725905
C	6.0	1.2503887725	2.0355895607	2.0817365502
H	1.0	0.4550768996	2.6664128275	1.7041010511
C	6.0	-1.3428238157	2.6972929091	-0.5106141165
H	1.0	-0.5965937522	2.7446610925	-1.2949704325
C	6.0	-2.2352185257	3.7390697469	-0.2753973009
H	1.0	-2.2018733774	4.6261993995	-0.8991438851
C	6.0	-3.1540704690	3.6156887056	0.7670463273
H	1.0	-3.8565446612	4.4134069029	0.9879331759
C	6.0	-3.1600377360	2.4456406951	1.5219022860
H	1.0	-3.8692539256	2.3307062751	2.3334614333
C	6.0	-2.2514490967	1.4243867594	1.2253794236
C	6.0	-2.2212372702	0.1251612081	1.9277868262
C	6.0	-3.1594109586	-0.2575275725	2.8937248217
H	1.0	-3.9288799388	0.4344881884	3.2162048607
C	6.0	-3.1203064765	-1.5433060011	3.4253557092
H	1.0	-3.8515231847	-1.8532342576	4.1654220926
C	6.0	-2.1358333123	-2.4264044798	2.9789707770
H	1.0	-2.0772817946	-3.4454482818	3.3470842590
C	6.0	-1.2110285584	-1.9736254138	2.0452141130
H	1.0	-0.4202068783	-2.6180433973	1.6776570552
O	8.0	-2.7843764289	-2.1741261640	-5.0250736956
H	1.0	-3.5493652003	-2.7457436936	-4.8442154133

[Ru(bpy)₂(bpy(O)₂)]

Nuclear Repulsion Energy (a.u.) = 4633.8470340

Total Energy (a.u.) = -1704.7001008

C₂ symmetry

RU	44.0	0.0000000000	0.0000000000	-0.0286525524
N	7.0	-1.0057937075	-0.8397379043	-1.6313589989
N	7.0	-1.3818471657	1.5321528992	0.1280234296
N	7.0	-1.2942307465	-0.7340123285	1.4677440707
O	8.0	-2.8067290357	-2.3755410481	-5.0275790513
C	6.0	-2.0550534195	-1.7079513749	-1.5602858085
H	1.0	-2.3785217601	-1.9628726287	-0.5539087518
C	6.0	-2.6832600045	-2.2502056726	-2.6480420943
H	1.0	-3.5167122931	-2.9345458320	-2.5170822574
C	6.0	-2.2680029779	-1.9156199393	-4.0043026584
C	6.0	-1.1511862943	-0.9802444541	-4.0320078785
H	1.0	-0.7881036257	-0.6827808441	-5.0097028773
C	6.0	-0.5689107903	-0.4777239436	-2.8912708837
C	6.0	-1.3883450386	2.6495863812	-0.6290195180
H	1.0	-0.6501960905	2.6742169642	-1.4214144385
C	6.0	-2.2781204841	3.6956719278	-0.4117402020
H	1.0	-2.2426194703	4.5702327877	-1.0530027049
C	6.0	-3.2042402342	3.5932064902	0.6284743262
H	1.0	-3.8990406249	4.4003531620	0.8397615180
C	6.0	-3.2228905715	2.4317678231	1.3938145727
H	1.0	-3.9320593796	2.3295309708	2.2072547474
C	6.0	-2.3124856542	1.4050075605	1.1195860499
C	6.0	-2.2832990795	0.1240134920	1.8468062198
C	6.0	-3.2091136322	-0.2339776781	2.8349900615
H	1.0	-3.9910983526	0.4570562024	3.1288084133
C	6.0	-3.1380844094	-1.4900111257	3.4276330985
H	1.0	-3.8569683626	-1.7792847801	4.1882014080
C	6.0	-2.1338216785	-2.3699902213	3.0186814633
H	1.0	-2.0457007538	-3.3665720521	3.4394064282
C	6.0	-1.2366950852	-1.9494855635	2.0451420068
H	1.0	-0.4456173108	-2.6009084662	1.6917165862

Nuclear Repulsion Energy (a.u.) = 5066.2073416

Total Energy (a.u.) = -1784.0710465

C₁ symmetry

RU	44.0	0.2508531077	-0.3754988842	0.6346036555
N	7.0	-0.7399172324	-0.7282272060	-1.1867308674
N	7.0	0.1850611787	1.5446963941	-0.2238994223
N	7.0	-1.4621540262	0.1267236049	1.7378239141
N	7.0	1.0821487615	0.2029627432	2.4730986203
N	7.0	0.3758638354	-2.3761459386	1.2573921071
N	7.0	2.0384650606	-0.9932108500	-0.2653780348
O	8.0	-2.6039122024	-1.2307391479	-4.8494497637
O	8.0	-0.0895711774	5.2484264687	-2.0533937877
C	6.0	-1.1800999260	-1.9277641194	-1.6283533355
C	6.0	-1.8062053378	-2.1096511352	-2.8440036653
C	6.0	-1.9973070421	-0.9973654170	-3.6858395159
C	6.0	-1.5411199184	0.2523798976	-3.2372354055
C	6.0	-0.9213129176	0.3547318751	-1.9896326129
C	6.0	-0.4201573015	1.6375607909	-1.4381237948
C	6.0	-0.5470775146	2.8571975436	-2.1072363155
C	6.0	-0.0369719639	4.0271898369	-1.5220922035
C	6.0	0.5894092100	3.9165281991	-0.2660293477
C	6.0	0.6716607457	2.6765807078	0.3326303846
C	6.0	-2.8273651513	-0.1551925972	-5.7747623961
C	6.0	-0.7176742716	5.4536440450	-3.3288369538
C	6.0	-2.7309348381	0.0701484761	1.2902547870
C	6.0	-3.8241241076	0.4350903832	2.0688722284
C	6.0	-3.5986976290	0.8854334257	3.3693396681
C	6.0	-2.2897613674	0.9501850816	3.8392517914
C	6.0	-1.2324467309	0.5654022250	3.0076795701
C	6.0	0.1854102374	0.5938165239	3.4227981880
C	6.0	0.6107563960	0.9917182920	4.6948719180
C	6.0	1.9683781997	0.9922977747	5.0026936472
C	6.0	2.8787166403	0.5918529210	4.0250281932
C	6.0	2.3933731187	0.2049237088	2.7802399929
C	6.0	-0.5127578979	-3.0112919827	2.0449386583
C	6.0	-0.3688931657	-4.3409710234	2.4269861140
C	6.0	0.7459787207	-5.0491001900	1.9791945416
C	6.0	1.6718829849	-4.3992540945	1.1674758419
C	6.0	1.4697393434	-3.0599938614	0.8169294456
C	6.0	2.3919705809	-2.2908928197	-0.0433151544
C	6.0	3.5572767420	-2.8259205593	-0.6030109821

C	6.0	4.3728021630	-2.0262137946	-1.3989118995
C	6.0	4.0035045260	-0.6995869162	-1.6201164352
C	6.0	2.8317604894	-0.2273577894	-1.0383790453
H	1.0	2.5040505970	0.7955025667	-1.1811077443
H	1.0	-1.0143771262	-2.7658446881	-0.9619609481
H	1.0	-2.1468802961	-3.0891185957	-3.1603942908
H	1.0	-1.6655335966	1.1304038118	-3.8553098735
H	1.0	-1.0369633911	2.9010185476	-3.0698047047
H	1.0	0.9952771779	4.8005531657	0.2128492282
H	1.0	1.1482125589	2.5638593542	1.2990947902
H	1.0	-3.3351466951	-0.6077917358	-6.6254570015
H	1.0	-1.8762121360	0.2791050985	-6.1019341146
H	1.0	-3.4689106888	0.6145425052	-5.3312904389
H	1.0	-0.6288960215	6.5214817438	-3.5246268872
H	1.0	-1.7758249826	5.1728006347	-3.2899061237
H	1.0	-0.1985242498	4.8913778405	-4.1128328229
H	1.0	-2.8582565200	-0.2840190777	0.2743437948
H	1.0	-4.8262637783	0.3668402888	1.6592925713
H	1.0	-4.4245664047	1.1817781337	4.0084030189
H	1.0	-2.0992500413	1.2997706320	4.8468421170
H	1.0	-0.1087139533	1.2973539765	5.4449251113
H	1.0	2.3064064087	1.2993233381	5.9874447908
H	1.0	3.9461837054	0.5759495467	4.2172866979
H	1.0	3.0653767676	-0.1130651060	1.9921765725
H	1.0	-1.3658078744	-2.4258324214	2.3673188165
H	1.0	-1.1173020675	-4.8046427967	3.0607912211
H	1.0	0.8940131378	-6.0885091628	2.2547404999
H	1.0	2.5439949243	-4.9354061859	0.8125524282
H	1.0	3.8297119600	-3.8589185438	-0.4227986542
H	1.0	5.2787489777	-2.4335990870	-1.8365226078
H	1.0	4.6079032855	-0.0380263763	-2.2314877748

Below is an example of some of the input parameters used in calculating vertical excitation energies using PCM solvent:

```
$CONTRL SCFTYP=RHF RUNTYP=ENERGY DFTTYP=B3LYP
      ISPHER=1 TDDFT=EXCITE PP=MCP $END
$TDDFT NSTATE=20 MAXVEC=12 $END
$PCM SOLVNT=12DCLET $END
$PCMCAV RADII=SUAHF $END
```