Electronic Supplementary Material (ESI) for Dalton Transactions
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Supplementary Information

Nitrosyl induces phosphorous-acid dissociation in ruthenium(II)†

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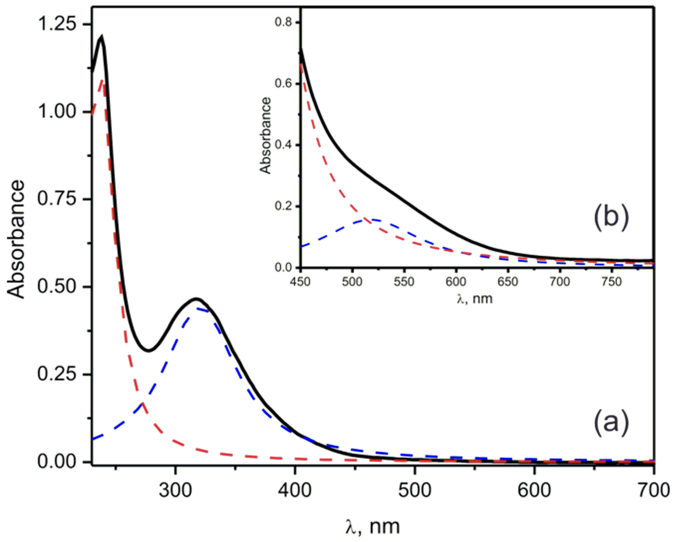

Fig SI 1 Electronic spectrum of *trans*-$[Ru(NO^{+})(NH_3)_4P(OH)_3]^{3+}$ at 0.5 mol L^{-1} CF_3COOH and 25±0.05°C (a) $C_{Ru} = 3.70\times10^{-4}$ mol L^{-1} and optical path of 1.0 cm (b) $C_{Ru} = 3.54\times10^{-3}$ mol L^{-1} and optical path of 5.0 cm.

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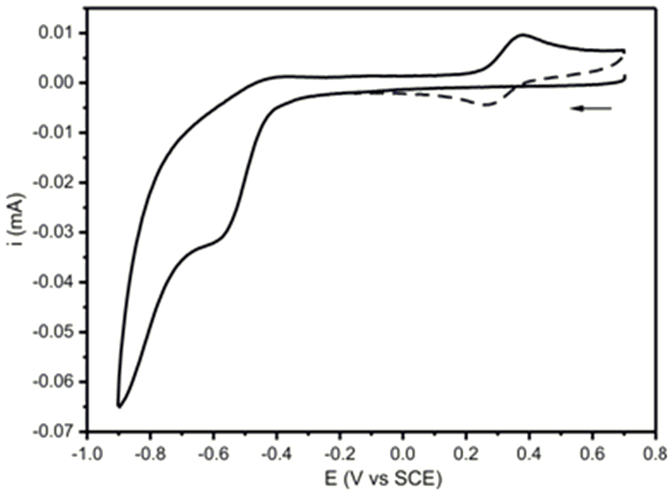

Fig. SI 2. Cyclic voltammogram of *trans*-$[Ru(NO^{+})(NH_3)_4P(OH)_3]^{3+}$ at 0.5 mol L^{-1} CF_3COOH, v = 50 mV s^{-1} and C_{Ru} = 1.0×10^{-3} mol L^{-1}, at 25±0.5°C; solid line: 1st cycle; dashed line: 2nd cycle.

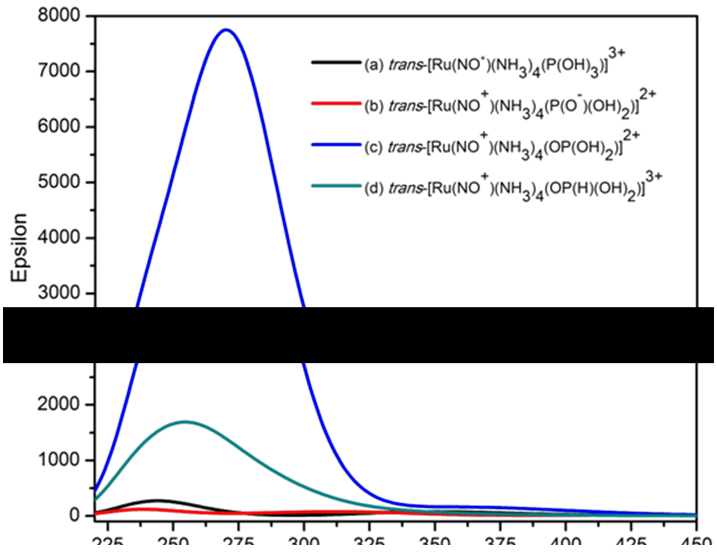

Fig. SI 3 Calculated TD-DFT electronic spectra for the structures A, B, C and D.

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Table SI 1 Geometric parameters (bond length, Å, and angle, °) for the phosphorous-acid complexes

(a)		(b)		(c)		(d)	
Ru-NO^+	1.840 Å	Ru-NO^+	1.856 Å	Ru-NO^+	1.802 Å	Ru-NO^+	1.798 Å
Ru-P	2.477 Å	Ru-P	2.467 Å	Ru-O	2.057 Å	Ru-O	2.071 Å
N O	1.126 Å	N O	1.127 Å	N O	1.132 Å	N O	1.129 Å
P-OH	1.596 Å	P-OH	1.618 Å	P-OH	1.653 Å	P-OH	1.600 Å
		P-O^-	1.535 Å	P-O	1.582 Å	P=O	1.543 Å
Ru-N O	178.94°	Ru-N O	178.02°	Ru-N O	179.13°	Ru-N O	179.31°
Ru-P-OH	108.55°	Ru-P-O^-	116.51°	Ru-O-P	139.19°	Ru-O=P	143.67°

Table SI 2 Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3), U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor

Atom	x	y	z	U(eq)
Ru	9182(1)	1324(1)	1385(1)	29(1)
P	6782(1)	545(1)	1275(1)	30(1)
O	11795(5)	2343(2)	1206(4)	56(1)
O(1)	7436(4)	-32(1)	565(3)	37(1)
O(2)	6021(5)	428(1)	2850(3)	50(1)
O(3)	4985(4)	813(1)	445(3)	42(1)
N(1)	9727(5)	1054(2)	-773(3)	38(1)
N(2)	6996(5)	1906(2)	601(4)	46(1)
N(3)	8441(5)	1504(2)	3557(4)	40(1)
N(4)	11066(5)	645(2)	2198(4)	38(1)
N(5)	10871(5)	1930(2)	1329(3)	35(1)
Zn	3706(1)	1321(1)	6157(1)	38(1)
Cl(1)	1357(2)	631(1)	5871(1)	50(1)
Cl(2)	3765(2)	1854(1)	4027(1)	46(1)
Cl(3)	6462(2)	858(1)	6653(2)	72(1)
Cl(4)	3023(2)	1983(1)	7979(1)	55(1)

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Table SI 3 Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3)

Atom	x	y	z	U(eq)
H(2)	6664	164	3250	75
H(3)	4318	536	130	64
H(1A)	10423	1335	-1202	46
H(1B)	8628	1009	-1265	46
H(1C)	10356	705	-760	46
H(2A)	6388	2063	1349	55
H(2B)	6179	1698	41	55
H(2C)	7502	2202	83	55
H(3A)	9394	1394	4156	48
H(3B)	7400	1296	3767	48
H(3C)	8215	1897	3660	48
H(4A)	12114	818	2572	46
H(4B)	11377	399	1478	46
H(4C)	10494	435	2887	46