

Supporting information

Bimetallic Ruthenium Complexes Bridged By Divinylphenylene Bearing Oligo(ethylene glycol)methylether: Synthesis, (Spectro)electrochemistry and Lithium Cation Effect

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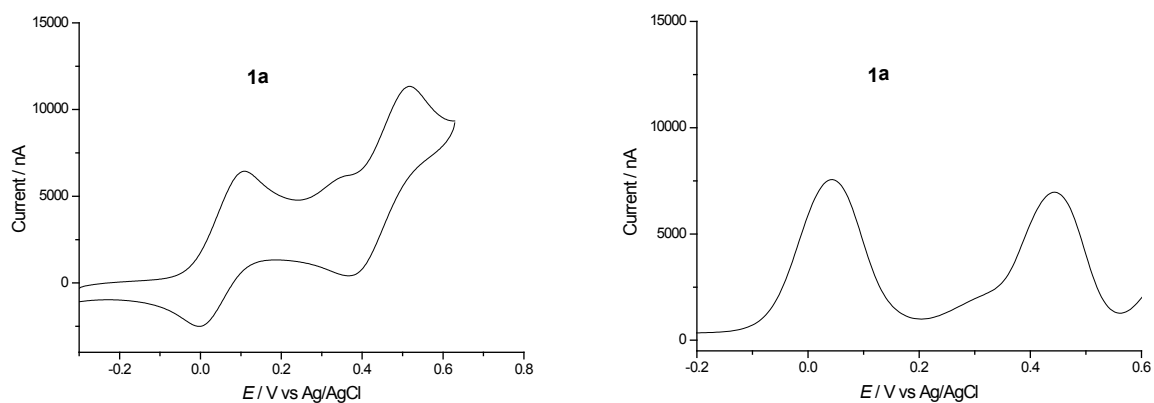


Figure S1. CV of complex **1a** in $\text{CH}_2\text{Cl}_2/[\text{N}^+\text{Bu}_4][\text{B}(\text{C}_6\text{F}_5)_4]$ at scan rate 100 mV s^{-1} (left). SWV of complex **1a** (scan rate: 100 mV s^{-1} , $f = 10 \text{ Hz}$, right).

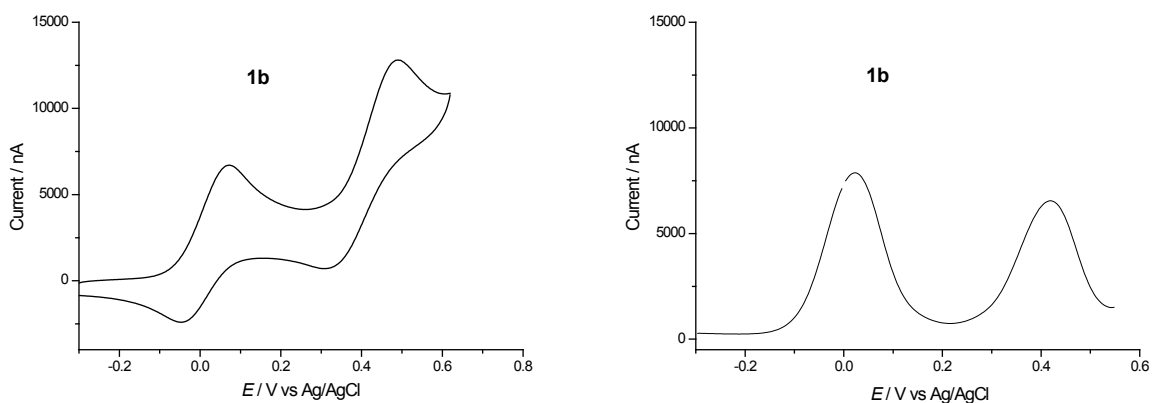


Figure S2. CV of complex **1b** in $\text{CH}_2\text{Cl}_2/[\text{N}^+\text{Bu}_4][\text{B}(\text{C}_6\text{F}_5)_4]$ at scan rate 100 mV s^{-1} (left). SWVs of complex **1b** (scan rate: 100 mV s^{-1} , $f = 10 \text{ Hz}$, right).

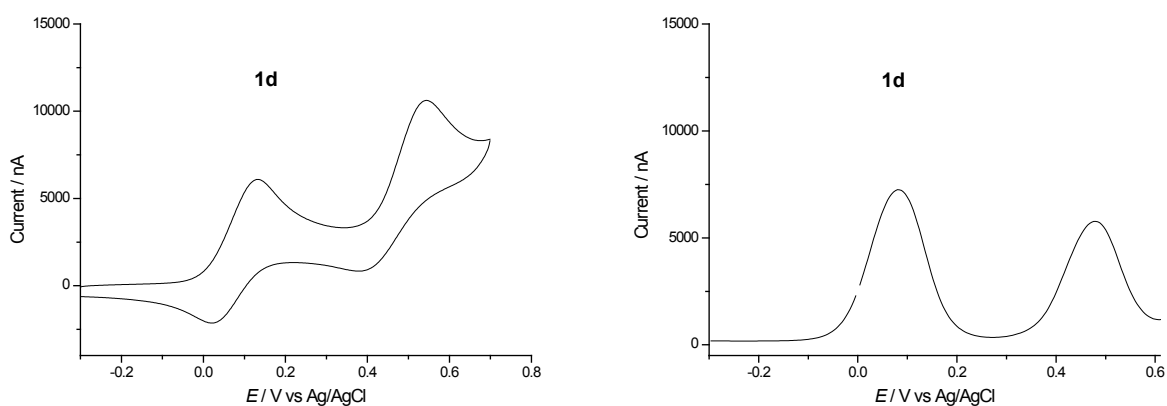


Figure S3. CV of complex **1d** in $\text{CH}_2\text{Cl}_2/[\text{N}^+\text{Bu}_4][\text{B}(\text{C}_6\text{F}_5)_4]$ at scan rate 100 mV s^{-1} (left). SWVs of complex **1d** (scan rate: 100 mV s^{-1} , $f = 10 \text{ Hz}$, right).

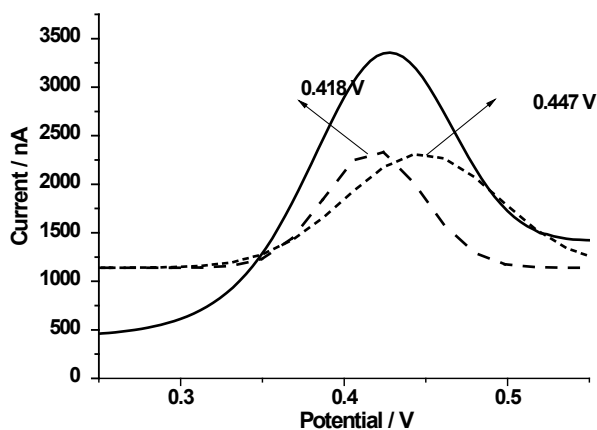


Figure S4. Deconvolution of the potential of complex **1g** after adding 1.0 eq Li⁺.

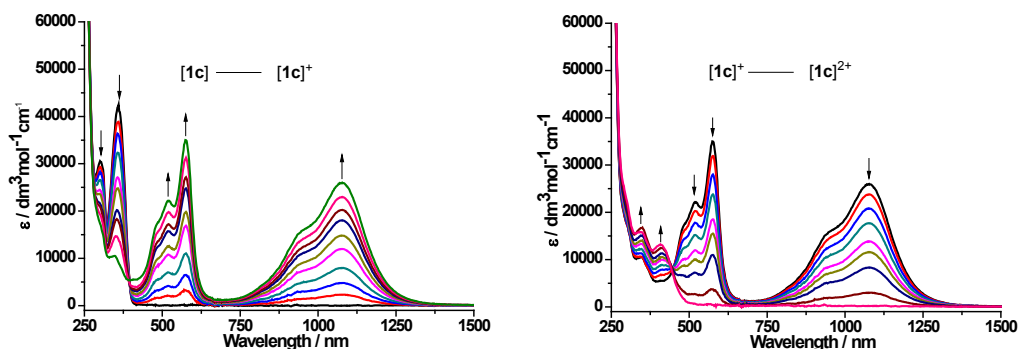


Figure S5. UV-Vis/near-IR spectra of complex **[1c]ⁿ⁺** (*n* = 0-2) in dichloromethane (2.0 mmol L⁻¹) collected during in situ oxidation in a spectroelectrochemical cell (0.05 M Bu₄N(C₆F₅)₄/CH₂Cl₂).

Table S1. Crystal data and structure refinement for complexes **1b**, **1e** and **1f**

	1b	1e
Formula	C ₃₆ H ₇₄ Cl ₂ O ₆ P ₆ Ru ₂	C ₃₂ H ₆₆ Cl ₂ O ₄ P ₆ Ru ₂
Fw	1061.81	973.71
Temp(K)	293(2)	293(2)
Wavelength(Å)	0.71073	0.71073
Crystal system	Monoclinic	Monoclinic
Space group	P2(1)/c	P2(1)/c
<i>a</i> (Å)	11.227(2)	14.560(3)
<i>b</i> (Å)	13.259(3)	21.265(4)
<i>c</i> (Å)	17.423(4)	15.947(3)
<i>α</i> (°)	90.00	90.00
<i>β</i> (°)	100.17(3)	101.77(3)
<i>γ</i> (°)	90.00	90.00
<i>V</i> (Å ³)	2552.8(9)	4833.7(17)
<i>Z</i>	2	4
Density (calculated)(Mg/m ³)	1.381	1.338

Absorption coefficient(mm ⁻¹)	0.921	0.963
F(000)	1100	2008
θ Range(°)	3.07-27.48	3.01-27.45
Index ranges	-13<= <i>h</i> <=14 -17<= <i>k</i> <=17 -22<= <i>l</i> <=22	-18<= <i>h</i> <=18 -27<= <i>k</i> <=27 -20<= <i>l</i> <=20
Reflections collected	21875	41196
Independent reflec.	5791	10964
	[R(int) = 0.0445]	[R(int) = 0.0684]
Refinement method	Full-matrix least-squares on F ²	Full-matrix least-squares on F ²
Data / restraints / parameters	5791 / 0 / 245	10964 / 0 / 416
Goodness-of-fit on F ²	1.070	1.053
Final <i>R</i> indices [<i>I</i> >2sigma(<i>I</i>)]	<i>R</i> ₁ = 0.0308 <i>wR</i> ₂ = 0.0668	<i>R</i> ₁ = 0.0579 <i>wR</i> ₂ = 0.1552
<i>R</i> indices (all data)	<i>R</i> ₁ = 0.0406 <i>wR</i> ₂ = 0.0752	<i>R</i> ₁ = 0.1084 <i>wR</i> ₂ = 0.1906
Largest diff. peak and hole	0.401 and -0.373 e. Å ⁻³	2.022 and -0.528 e. Å ⁻³

Table S2 Selected bond lengths (Å) and angles (deg) for complex **1b**, and **1e**

1b		1e	
Ru(1)-P(1)	2.3732(9)	Ru(1)-P(1)	2.360(2)
Ru(1)-Cl(1)	2.4758(9)	Ru(1)-Cl(1)	2.4660(18)
Ru(1)-C(1)	2.096(2)	Ru(1)-C(10)	2.111(5)
C(1)-C(2)	1.341(3)	C(10)-C(11)	1.324(8)
C(2)-C(3)	1.473(3)	C(13)-C(12)	1.426(8)
C(5)-O(3)	1.381(3)	O(2)-C(17)	1.385(6)
C(2)-C(1)-Ru(1)	130.7 (2)	C(11)-C(10)-Ru(1)	130.9(4)
C(1)-C(2)-C(3)	127.6(2)	C(10)-C(11)-C(12)	126.9(6)
C(5)-C(3)-C(2)	121.1(2)	C(17)-C(12)-C(11)	121.3(5)
O(3)-C(5)-C(3)	115.8(2)	O(2)-C(17)-C(12)	118.5(5)