Study of electrospun nanofibers loaded with Ru(II) phenanthroline complexes as a potential material for use in dye-sensitized solar cells (DSSCs).

Luis Jesús Villarreal Gómez^{a,b*}, Ana Leticia Iglesias ^{a,b*}, Valentín Miranda Soto^c, Amelia Livas Sarabia^d Ricardo Valdez Castro^d, Eduardo Alberto López Maldonado^b, Mercedes Teresita Oropeza Guzman^c, Christian Alfonso Romero Soto^{a,c}, Eder German Lizarraga Medina^a, Jorge Luis Vazquez Arce^d

^aFacultad de Ciencias de la Ingeniería y Tecnología, Universidad Autónoma de Baja California, Unidad Valle de las Palmas, Tijuana, Baja California, México

^bFacultad de Ciencias Químicas e Ingeniería, Universidad Autónoma de Baja California, Unidad Otay, Tijuana, Baja California, México

^cCentro de Graduados e Investigación en Química, Instituto Tecnológico de Tijuana, Tijuana, Baja California, México

^dCentro de Nanociencias y Nanotecnología, Universidad Nacional Autónoma de México.



Figure S1. Full ¹H NMR of [RuCl₂(*p*-cymene)]₂ in CDCl₃(400 MHz)



HSQC		COSY	COSY		$\begin{array}{c} 3\\ 8 16 \leftrightarrow 120.0 \end{array}$
Group CH=N		0.90	2.62		2
9.99	156.0	6.14	6.38		↔156.0
Grupos CH aromatic		8.16	8.94		2
6.14	83.7		9.99		8.30 [→] 129.9
6.38	85.9	¹ H- ¹³ C	C HMBC		↔138.7
8.16	126.3	3			$3 \leftrightarrow 1.45$ 0
8.30	127.4	0.90~21.6		143.0	
8.94	138.7	↔30.3		8.94↔127.4	
Grupos Alkyl CH ₃		3	3		3
0.90	21.6	\leftrightarrow	103.9		⇔145.0
0.70	10.1	3 2 17↔	og 75		3 ↔156 0
2.17	18.1	2.1/**	03.73		2
Grupos CH alkyl		$\stackrel{2}{\leftrightarrow}$	$\stackrel{2}{\leftrightarrow}$ 102 6		9 99↔126 3
2.62	30.3	2	102.0		3
<i>Ispo</i> carbons		2.62↔	2.62⇔21.6		↔138.7
102.6		3			3
102.0		\leftrightarrow	⇔85.9		↔145.0
103.9		2	2		
129.0		\leftrightarrow	↔103.9 d		
145.0		2 6 14↔	2 6 14↔85 0		¹ H- ¹⁵ N HMBC
		0.14	0.5.7		11- 13 IIIVIDC
		\leftrightarrow	103.9		8.16↔ 235.8

	10019	0.00 -00.0
Figure S3. ¹ H RMN data in red	, ¹³ C NMR data in blue,	, and ¹⁵ N NMR data in black.





Figure S4. Partial ¹H-¹H gCOSY NMR of Ru-1 in DMSOd₆ (400 MHz)

Figure S5. Partial ¹H-¹H gCOSY NMR of Ru-1 in DMSOd₆ (400 MHz)



Figure S6. Partial ¹H-¹H gCOSY NMR of Ru-1 in DMSOd₆ (400 MHz)



Figure S7. Partial ¹H-¹³C gHSQC NMR of **Ru-1** in DMSO d_6 (400 MHz)



Figure S8. Partial ¹H-¹³C gHSQC NMR of Ru-1 in DMSOd₆ (400 MHz)



Figure S9. Partial ¹H-¹³C gHSQC NMR of Ru-1 in DMSOd₆ (400 MHz)



Figure S10. Full ¹H-¹³C HMBC NMR of Ru-1 in DMSOd₆. (400 MHz)



Figure S11. Partial ¹H-¹³C HMBC NMR of Ru-1 in DMSOd₆ (400 MHz)



Figure S12. Full ¹H-¹³C HMBC NMR of Ru-1 in DMSOd₆ (400 MHz)



Figure S13. HRMS of compound Ru-1.



gure S14. HRMS for Ru-1 (above) and simulated spectrum (below), for [M + Na]⁺ for compound Ru-1



Figure S15. Full ¹H NMR (top) and ¹³C NMR (bottom) of complex Ru-2 in DMSOd₆ (400 MHz)



HSQC	138.9	3	3	
	144.7	↔83.5	↔150.2	
Group CH=N	145.9	2	3	
	145.9	⇔85.8	9.12↔144.7	
9.43 150.2		3	3	
9.88 155.6	COSY	⇔103.4	₩145.9	
Group CH aromatic	0.89 2.57	3 ()7⇔20 2	3 ⇔155 (
6 05 82 5	6.05 6.27	0.2/~ 30.3	×155.0	
0.03 85.3	7 81 8 41	∠ ↔83.5	0 43↔125 8	
6.27 85.8	0.42	3	3	
6.99 100.6	9.43	↔85.8	↔134 7	
7.81 125.8	8.09 9.12	3	3	
8.09 124.6	9.88	↔102.3	↔138.9	
8.41 134.7	¹ H- ¹³ C HMBC	3	2	
0.12 123.0	3	6.94 ↔100.6	9.88↔124.6	
9.12 155.9	0.89↔21.5	3	3	
Group alkyl CH ₃	2	↔123.0	↔133.9	
0.89 21.5	↔30.3	3	3	
2.16 18.1	3	6.99↔123.0	↔145.9	
Group CH alkyl	↔103.4	2		
2.57 20.2	3	↔132.1	1H_15N HMBC	
2.37 30.3	2.16↔83.5	3		
Ipso carbons	2	↔134.7	$600 \leftrightarrow 684$	
102.6	↔102.6	3	0.99** 00.4	
103.4	2	↔138.9	7 81↔ 234	
123.0	2.57~21.5	3	3	
123.0	3	7.81↔132.1	$8.09 \leftrightarrow 236.4$	
132.1	~85.8	2	0.07 250.4	
	2	↔150.2		

Figure S16. ¹ H RMN data in red, $\stackrel{13}{_{3}}C^{103}MR$ data in blue, and ¹⁵ N NMR data in black 6 05 \leftrightarrow 18 1



Figure S17. Partial ¹H-¹H gCOSY NMR of Ru-2 in DMSOd₆ (400 MHz).



Figure S18. Partial ¹H-¹H gCOSY NMR of Ru-2 in DMSOd₆ (400 MHz)



Figure S19. Partial ¹H-¹³C NMR HSQC of Ru-2 in DMSOd₆(400 MHz)



Figure S20. Partial ¹H-¹³C NMR HSQC of Ru-2 in DMSOd₆ (400 MHz)



Figure S21. Partial ¹H-¹³C NMR HMBC of Ru-2 in DMSOd₆ (400 MHz)



Figure S22. Partial ¹H-¹³C NMR HMBC of Ru-2 in DMSOd₆ (400 MHz)



Figure S23. HRMS of compound Ru-2.



Figure S24. HRMS for Ru-2 (above) and simulated spectrum (below), for $[M + Na]^+$ for complex Ru-2.



Figure S25. FT-IR spectrum of 1,10-phenanthroline (phen).



Figure S26. FT-IR spectrum of 5-amino-1,10-phenanthroline (5-phen).



Figure S27. FT-IR spectrum of Ru-1 complex



Figure S28. FT-IR spectrum of Ru-2 complex.