

The spin state of a charged non-IPR Fullerene: The stable radical cation of

Sc₃N@C₆₈

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Table S1. Redox potentials and electrochemical energy gap $\Delta E_{\text{gap,ec}}$ (V) of Sc₃N@C₆₈ in comparison with the data of Sc₃N@C₈₀ (*I_h*)

sample	Redox potential (V vs Fc/Fc ⁺)				Energy gap $\Delta E_{\text{gap,ec}}$ (V) ^b	Reference
	$E_{1/2}$, red(1) ^a	$E_{1/2}$, red(2) ^a	$E_{1/2}$, ox(1)	$E_{1/2}$, ox(2)		
Sc ₃ N@C ₆₈	-1.38 ^a	-1.98	0.33	0.85	1.71	this work
	-1.24	-1.62	0.62	-	1.86	17
Sc ₃ N@C ₈₀ (<i>I_h</i>)	-1.26	-1.62	0.59	-	1.85	21
	-1.22	-1.59	0.62	-	1.84	22

^a Because of the obvious irreversibility of the two reduction steps, the formal potential of the reduction of Sc₃N@C₆₈ is taken by the half-peak potential.

^b Electrochemical gap is calculated as $E_{1/2, \text{ox}(1)} - E_{1/2, \text{red}(1)}$.

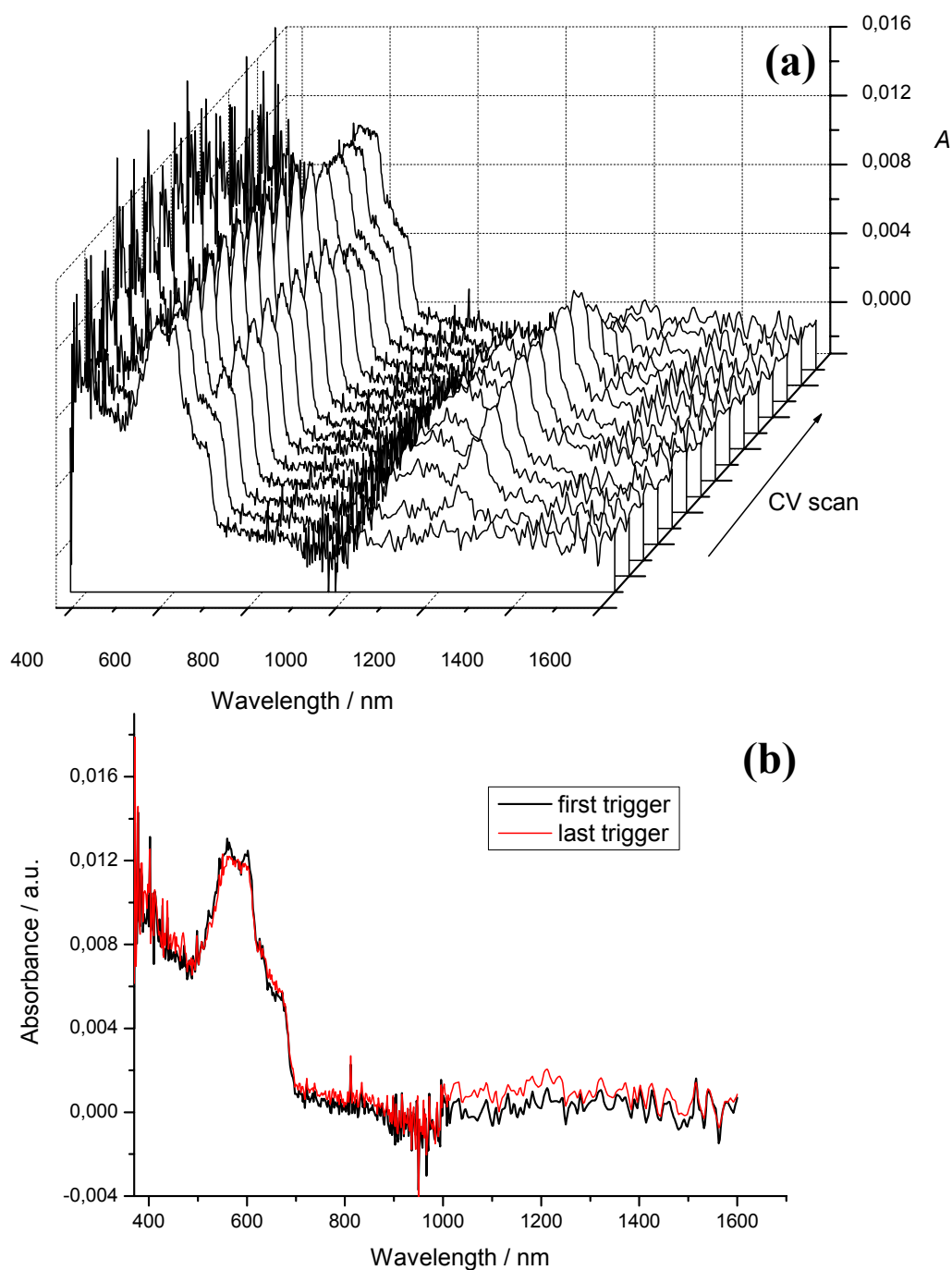


Figure S1. *In situ* spectroelectrochemistry of Sc₃N@C₆₈ oxidation in 0.2 M TBAPF₆/o-DCB: a) UV-Vis-NIR spectra (in a 3D plot) recorded during the cyclic voltammetric scan in the potential range from -0.2 to 0.8 V vs. Fc/Fc⁺ (scan rate: 3 mV s⁻¹). b) The spectra of Sc₃N@C₆₈ recorded before (black line) and after (red line) CV scan.