

Supporting Information for

**Coordination chemistry of sterically encumbered
pyrrolyl ligands to chromium(II):
Mono(pyrrolyl)chromium and diazachromocene
formation**

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1. UV/vis Spectroscopy on diazachromocenes

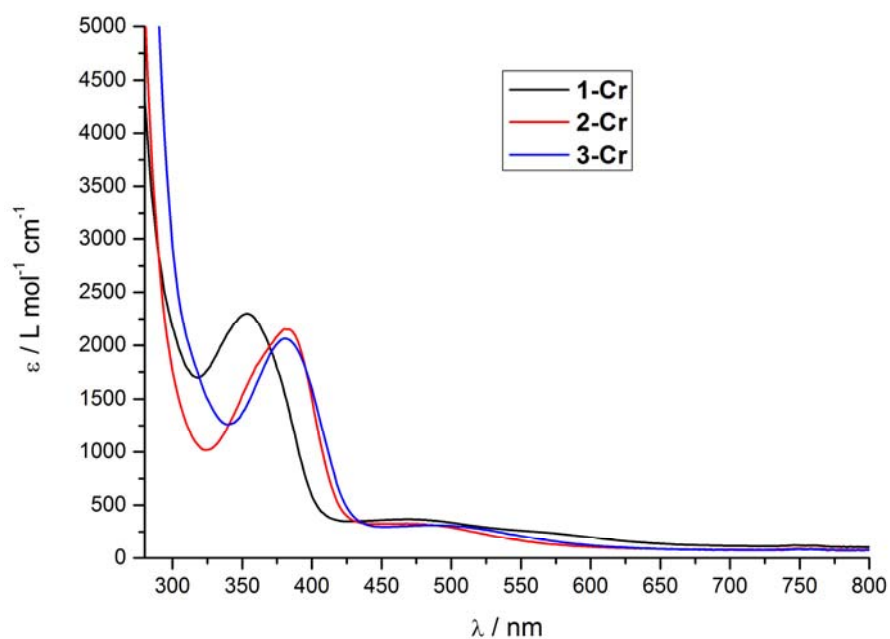


Figure S1. UV/vis spectra of **1-Cr**, **2-Cr** and **3-Cr** recorded in hexane at ambient temperature.

Table S1. UV-vis spectra of diazachromocenes

Compound ^a	$\lambda_{\text{max}} / \text{nm} [\epsilon / \text{L mol}^{-1} \text{cm}^{-1}]$
1-Cr	354 [2300], 470 [370]
2-Cr	382 [2150], 470 [325]
3-Cr	380 [2060], 488 [310]

^a UV-vis spectra recorded in hexane solution at ambient temperature.

2. UV/vis Spectroscopy on mono(pyrrolyl)chromium complexes

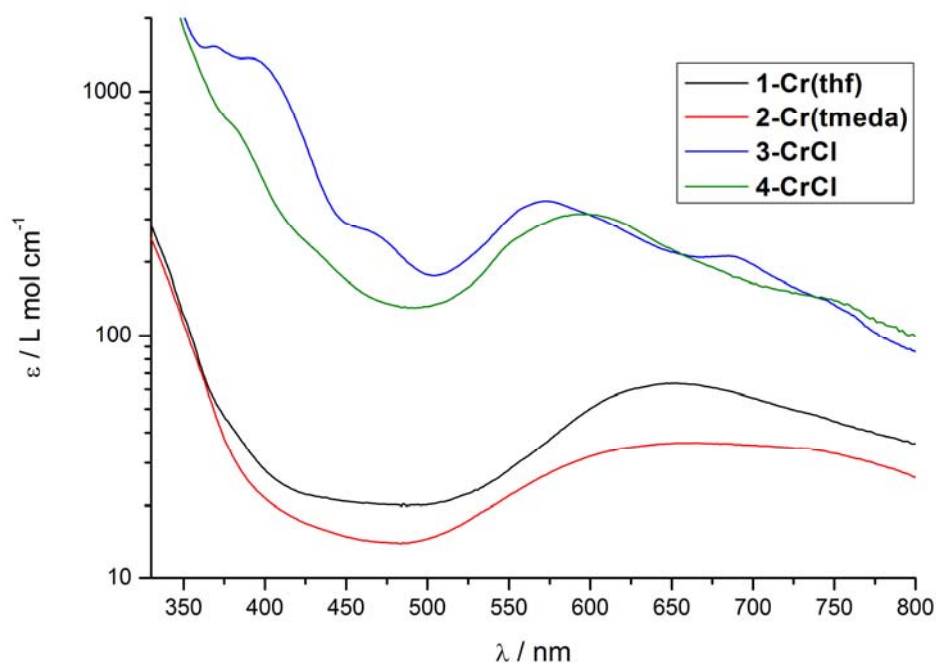


Figure S2. UV/vis spectra of **1-Cr(thf)**, **2-Cr(tmeda)**, **3-CrCl** and **4-CrCl** recorded at ambient temperature.

Table S2. UV-vis spectra of **1-Cr(thf)**, **2-Cr(tmeda)**, **3-CrCl** and **4-CrCl**^a

Compound	λ_{\max} / nm [ϵ / L mol ⁻¹ cm ⁻¹]	solvent
1-Cr(thf)	654 [64]	THF
2-Cr(tmeda)	666 [36]	THF
3-CrCl	594 [315], 748 [142]	hexane
4-CrCl	368 [1530], 390 [1370], 463 (sh) [270], 573 [357], 684 [212]	hexane

^a UV-vis spectra recorded at ambient temperature.

3. Conditions for catalytic testing

	Autoklav: 30 bar ethylene 50°C			
	ratio: Cr:Ligand:Cl:Al		Cr:Ligand:Cl:Al	
	1:1:1:100		1:1:3:30	
	Trial 1 (MAO)		Trial 2 (TEA)	
Complex: 2-Cr(tmeda)				
	Complex:	12mg	Complex:	12mg
	DoTriMAC:	no	DoTriMAC:	16mg
	MAO (in toluene): (ca. 1.5 mol/L)	2,0mL	TEA (in toluene): (ca. 1.9 mol/L)	0,5mL
	toluene:	ca. 98mL	toluene:	ca.100mL
Complex: 3-CrCl				
	Complex:	10mg	Complex:	10mg
	DoTriMAC:	no	DoTriMAC:	16mg
	MAO (in toluene): (ca. 1.5 mol/L)	2,0mL	TEA (in toluene): (ca. 1.9 mol/L)	0,5mL
	toluene:	ca. 98mL	toluene:	ca.100mL
Complex: 4-CrCl				
	Complex:	10mg	Complex:	10mg
	DoTriMAC:	no	DoTriMAC:	16mg
	MAO (in toluene): (ca. 1.5 mol/L)	2,0mL	TEA (in toluene): (ca. 1.9 mol/L)	0,5mL
	toluene:	ca. 98mL	toluene:	ca.100mL
	DoTriMAC: Dodecyltrimethylammoniumchloride			
	MAO: Methylaluminoxane			
	TEA: Trimethylaluminum			