

Redox chemistry of Pt(II) complex with non-innocent NHC bis(phenolate) pincer ligand: electrochemical, spectroscopic and computational aspects

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Supplementary Materials

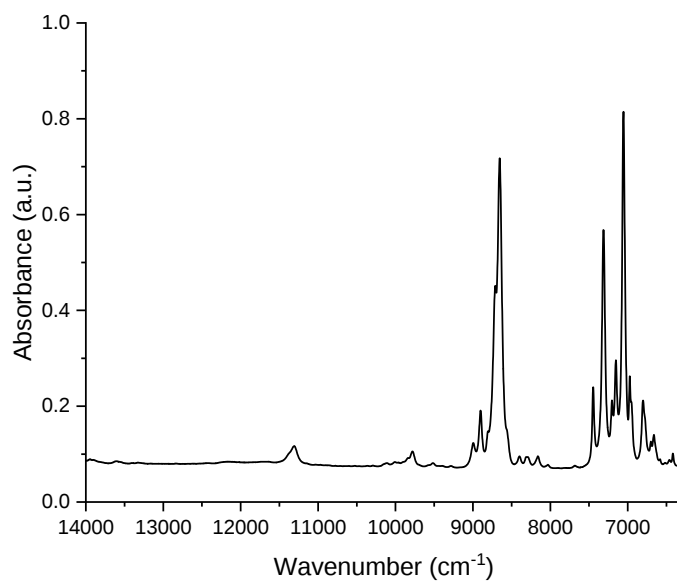


Figure S1. NIR spectrum of CH_2Cl_2 at 298 K, $l = 1$ cm.

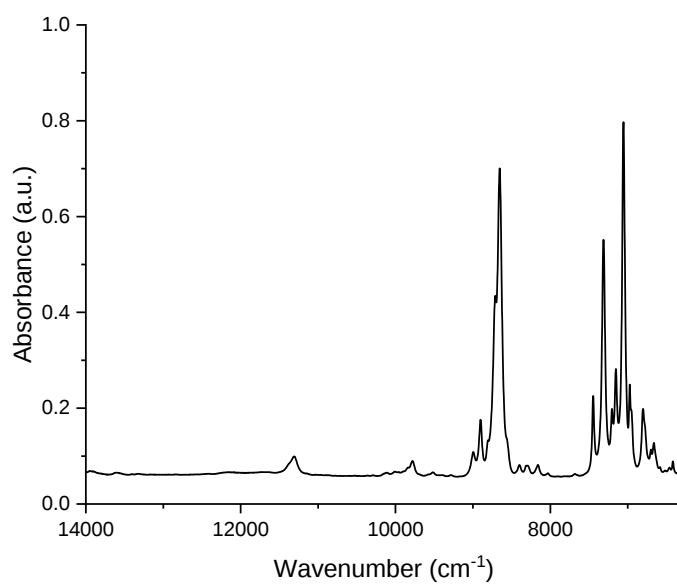


Figure S2. NIR spectrum of $\text{Pt}(\text{L})\text{Py}$ ($c = 0.1$ mM) in CH_2Cl_2 at 298 K, $l = 1$ cm.

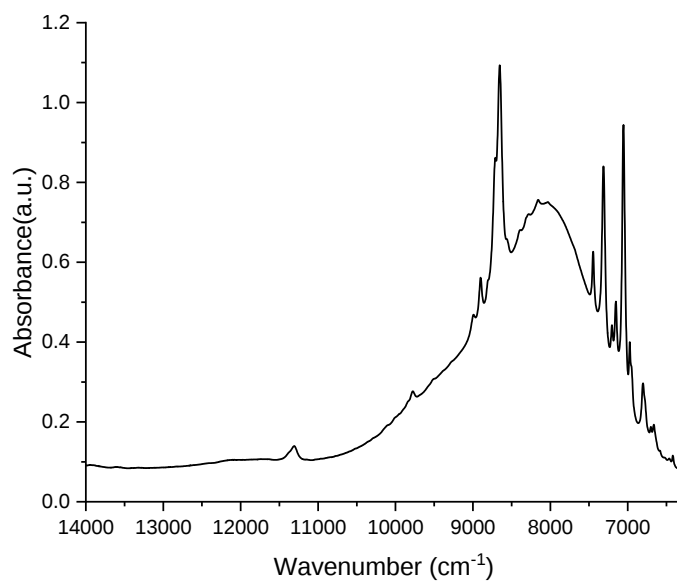


Figure S3. NIR spectrum of [Pt(L)Py][BF₄] (*c* = 0.1 mM) in CH₂Cl₂ at 298 K, *l* = 1 cm.

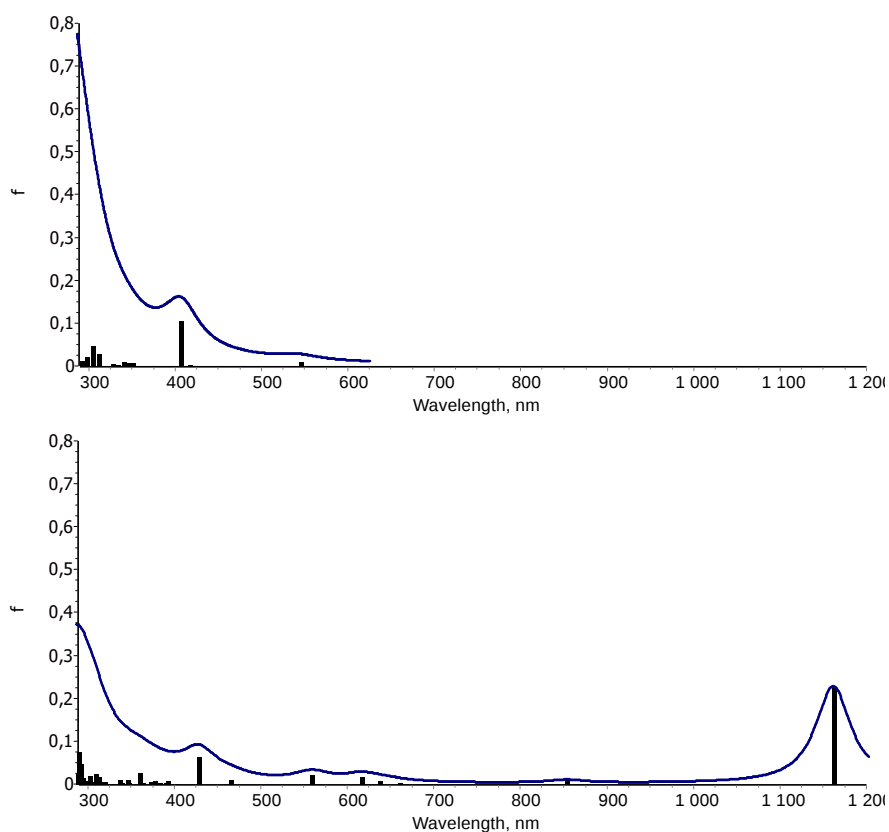
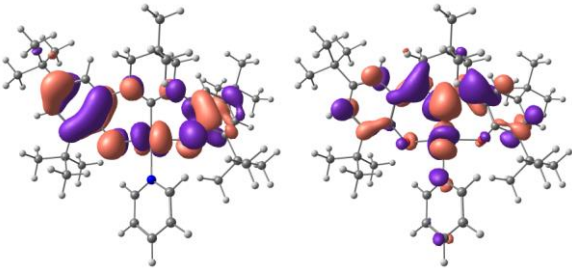
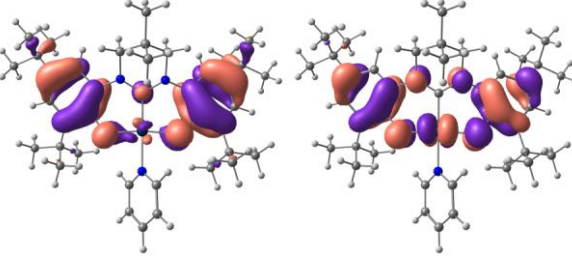
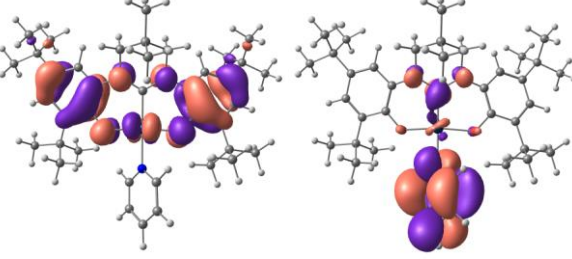
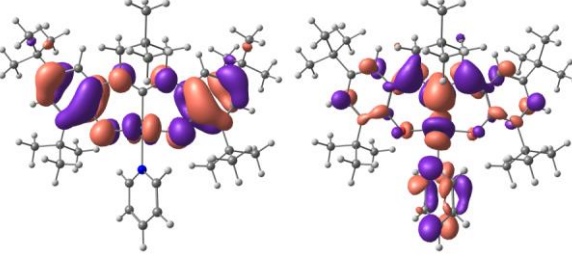


Figure S4. The calculated absorption spectra for Pt(L)Py (top graph) and [Pt(L)Py][BF₄] (bottom graph). The vertical lines showing the position of electronic transitions and their intensity (*f* – oscillator strength) were broadened by the Lorentz function.

Table S1. Selected TD-DFT-calculated excitation energies (absorption wavelengths), oscillator strengths, and main compositions of the most important electronic transitions for Pt(L)Py and [Pt(L)Py][BF₄].

λ	f	Transition
Pt(L)Py		
407	0.10	 HOMO $\rightarrow$ LUMO+2 (95%)
[Pt(L)Py][BF₄]		
1162	0.23	 β: HOMO $\rightarrow$ LUMO (97%)
429	0.06	 α: HOMO $\rightarrow$ LUMO (58%)  α: HOMO $\rightarrow$ LUMO+1 (32%)

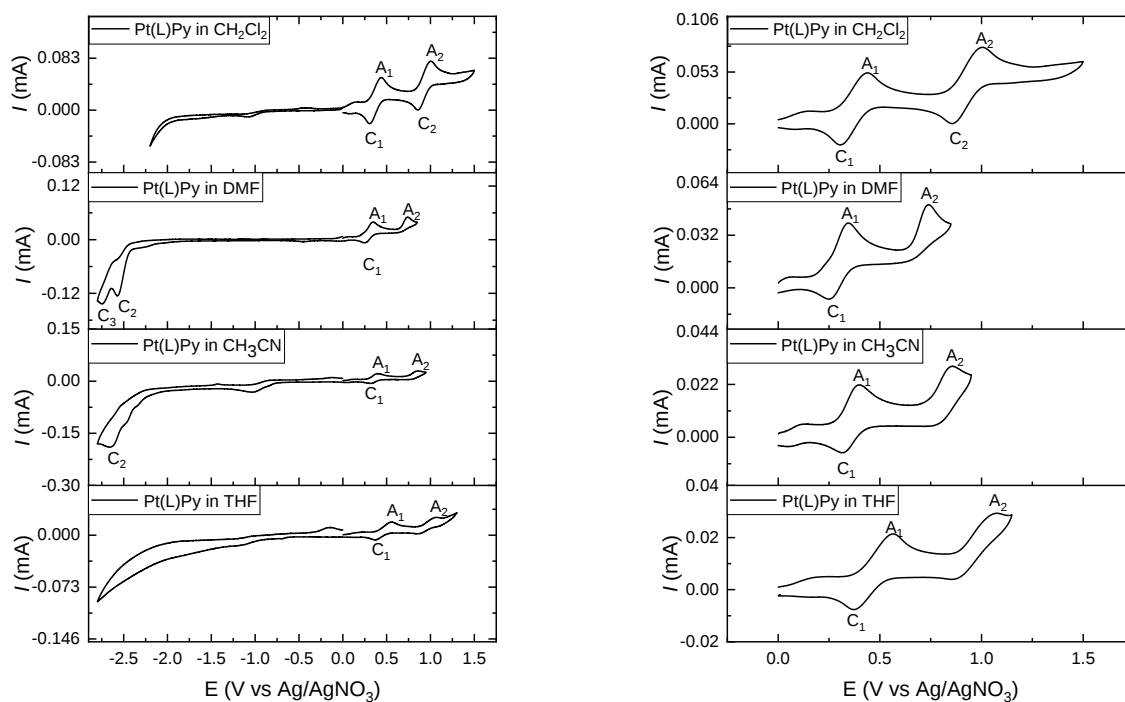


Figure S5. CV-curves recorded from a solution containing complex **Pt(L)Py** in different solvents ($c = 5$ mM) in the presence of $(n\text{-Bu}_4\text{N})\text{BF}_4$ (0.1 M) at the scan rate of $100 \text{ mV}\cdot\text{s}^{-1}$ on the GC working electrode ($T = 298 \text{ K}$).

Table S2. Peak potentials* on the CV-curves of complex **Pt(L)Py** obtained in different solvents.

Solvent	Cathodic peaks	$E_{\text{p}^{\text{red}}}$, V	Anodic peaks	$E_{\text{p}^{\text{ox}}}$, V
CH₂Cl₂	C ₁	+0.85	A ₁	+0.44
	C ₂	+0.30	A ₂	+1.01
DMF	C ₁	+0.24	A ₁	+0.34
	C ₂	-2.57	A ₂	+0.73
	C ₃	-2.74		
CH₃CN	C ₁	+0.32	A ₁	+0.40
	C ₂	-2.65	A ₂	+0.85
THF	C ₁	+0.36	A ₁	+0.55
			A ₂	+1.07

* The mentioned potentials are referred to the Ag/AgNO_3 (0.01 M solution in CH_3CN).