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

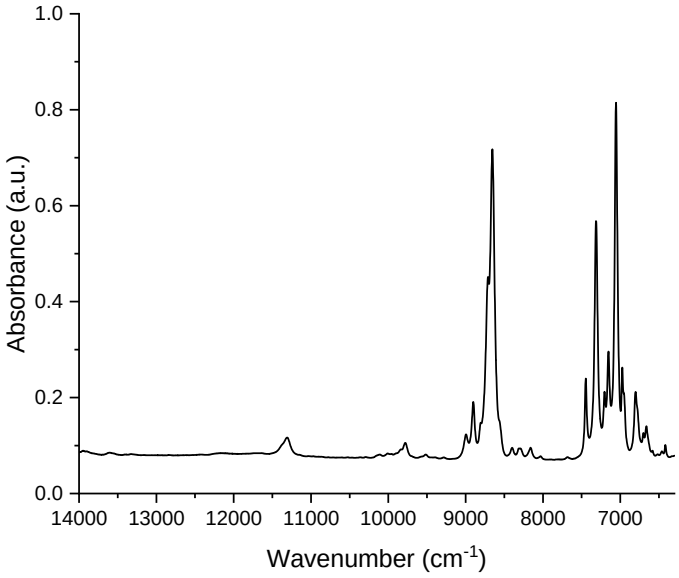


Figure S1. NIR spectrum of CH_2Cl_2 at 298 K, l = 1 cm.

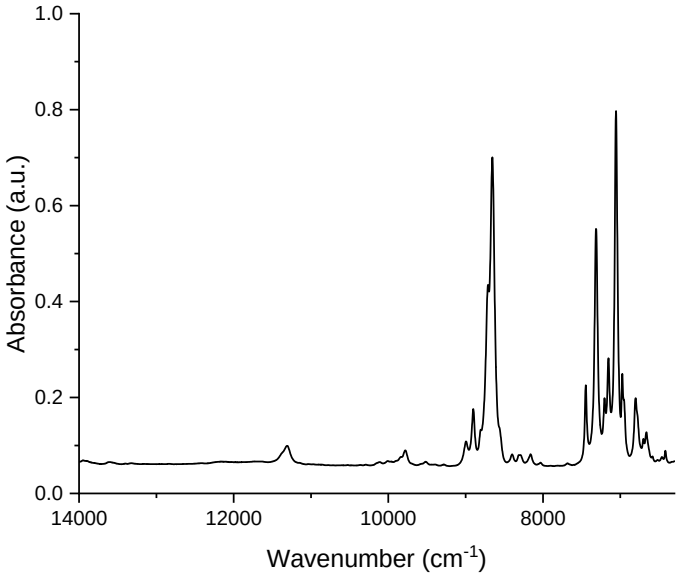


Figure S2. NIR spectrum of **Pt(L)Py** (c = 0.1 mM) in CH_2Cl_2 at 298 K, l = 1 cm.

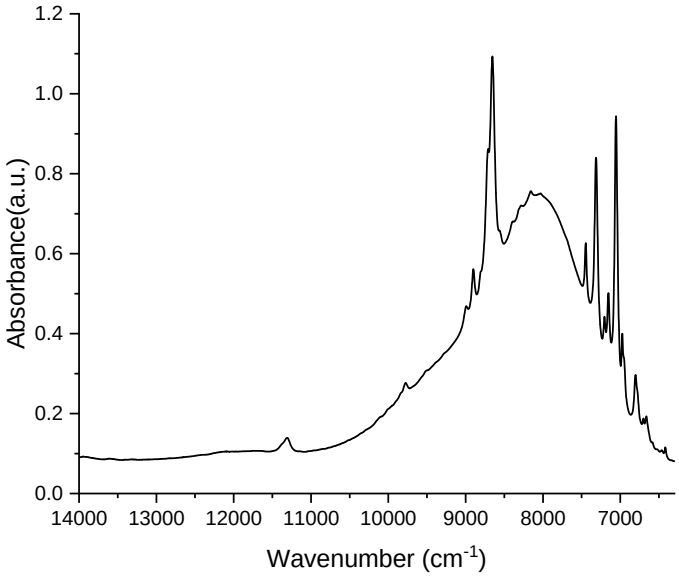


Figure S3. NIR spectrum of **[Pt(L)Py][BF$_4$]** (c = 0.1 mM) in CH_2Cl_2 at 298 K, l = 1 cm.

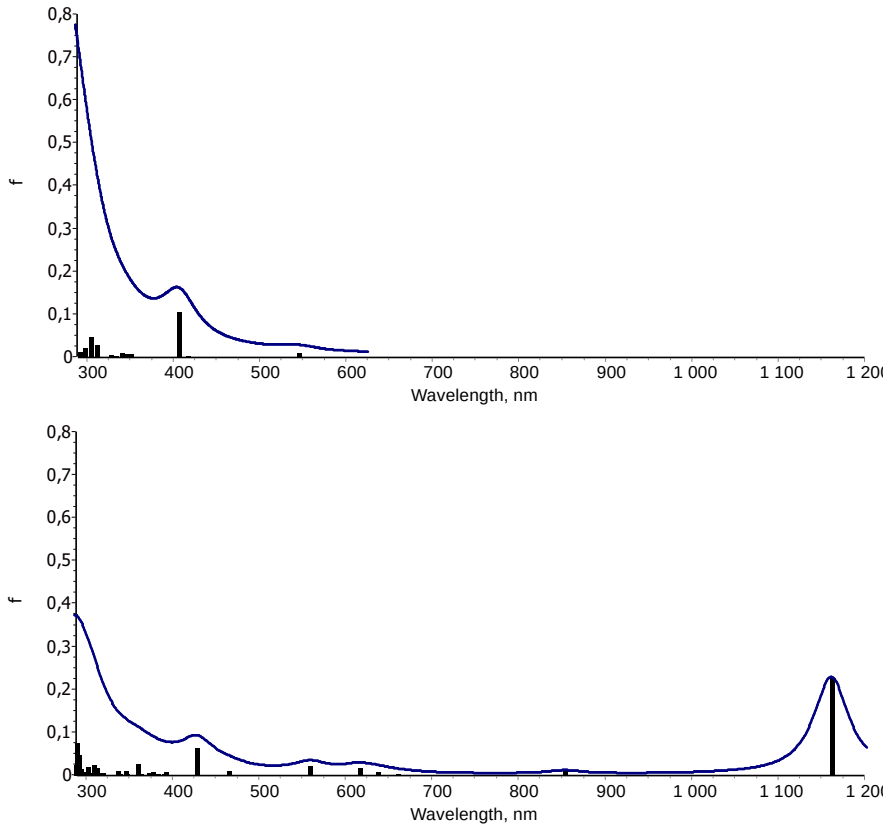
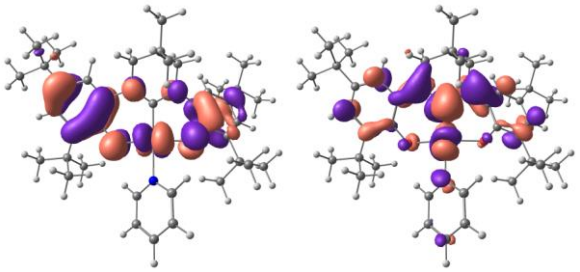
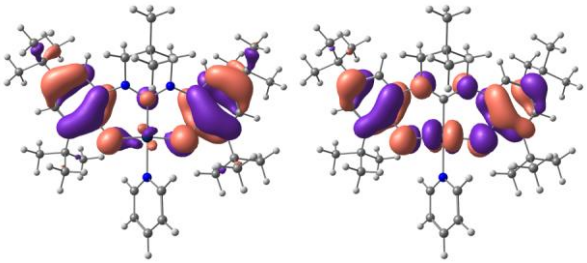
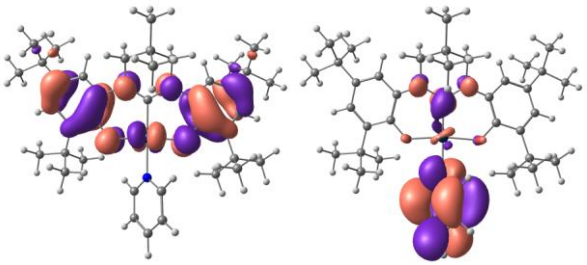
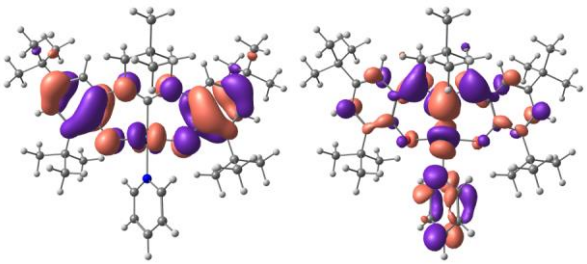


Figure S4. The calculated absorption spectra for **Pt(L)Py** (top graph) and **[Pt(L)Py][BF$_4$]** (bottom graph). The vertical lines showing the position of electronic transitions and their intensity (*f* – oscillator strength) were broadened by the Lorentz function (f.w.h.m. = 50 nm).

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][BF$_4$]**.

λ	f	Transition
Pt(L)Py		
407	0.10	 HOMO → LUMO+2 (95%, contour value = 0.03)
[Pt(L)Py][BF_4]		
1162	0.23	 β: HOMO → LUMO (97%, contour value = 0.03)
429	0.06	 α: HOMO → LUMO (58%, contour value = 0.03)  α: HOMO → LUMO+1 (32%, contour value = 0.03)

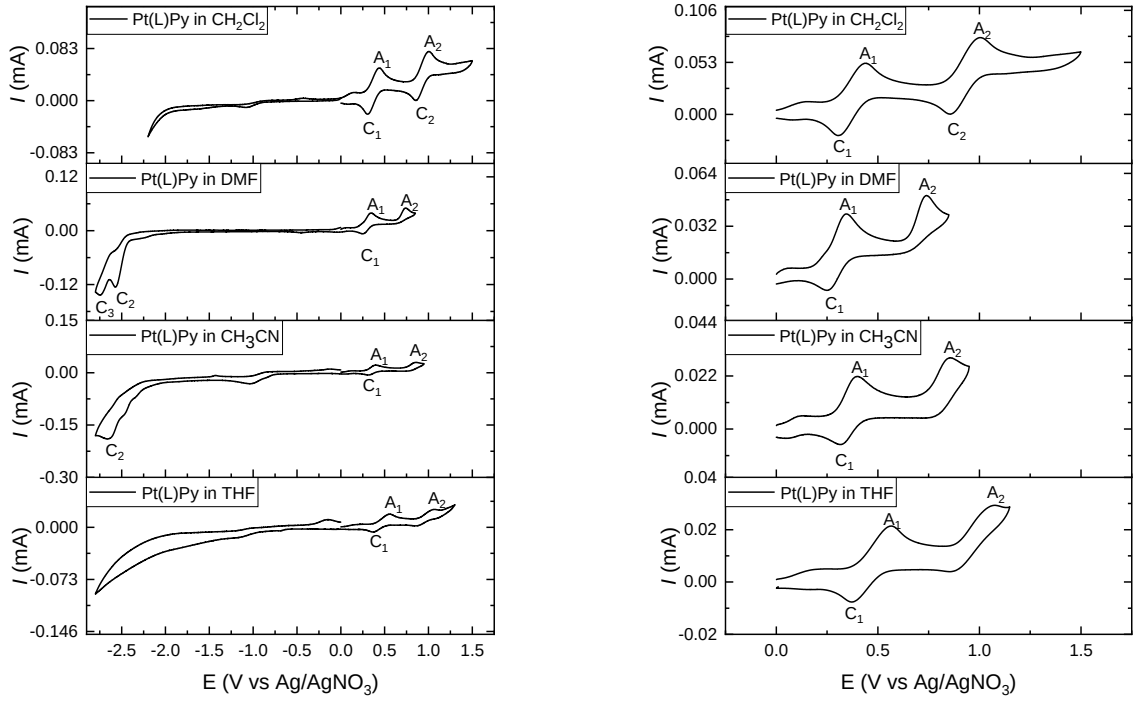


Figure S5. CV-curves recorded from a solution containing complex **Pt(L)Py** in different solvents (c = 5 mM) in the presence of (*n*-Bu$_4$N)BF$_4$ (0.1 M) at the scan rate of 100 mV·s^{-1} on the GC working electrode (T = 298 K).

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

Solvent	Cathodic peaks	E_p^{red}, V	Anodic peaks	E_p^{ox}, V
CH_2Cl_2	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		
CH_3CN	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 $Ag/AgNO_3$.

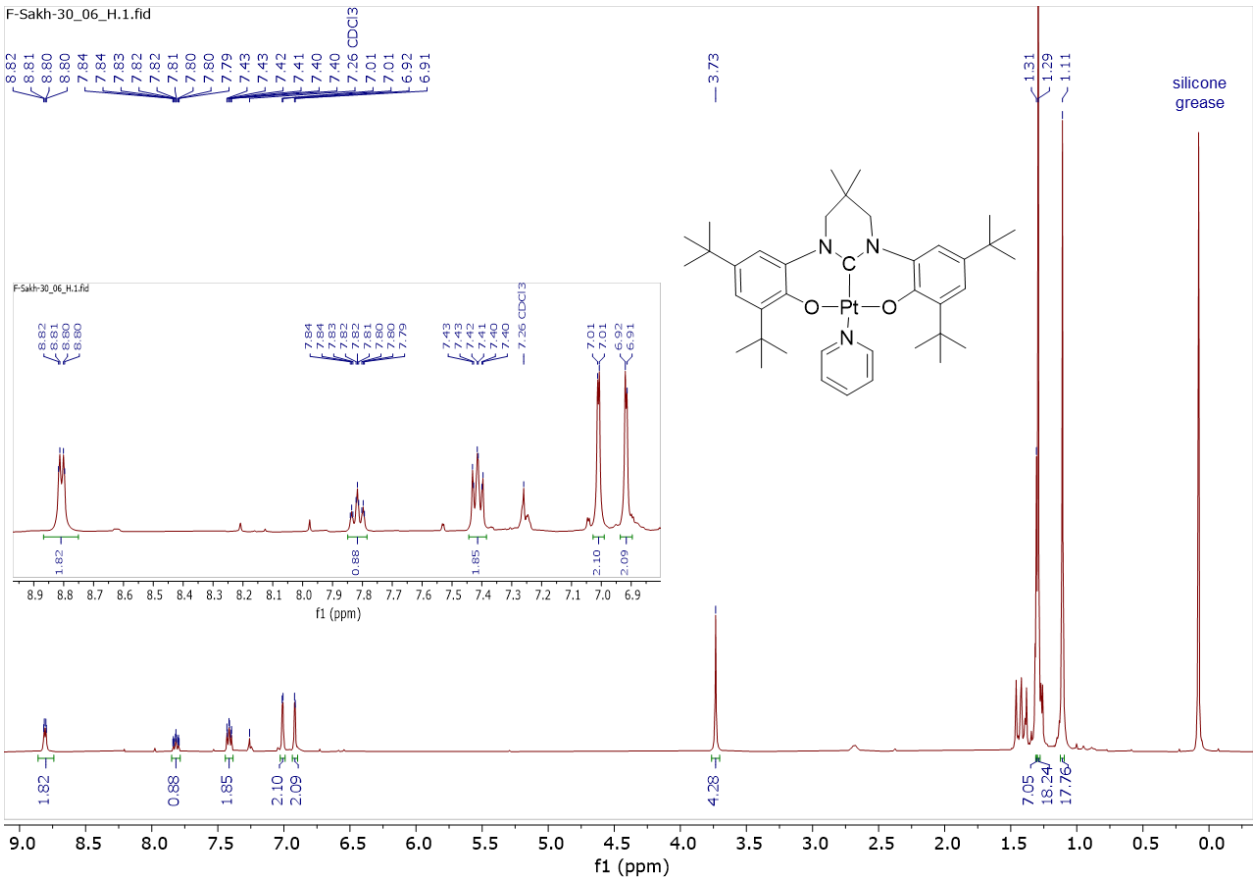


Figure S6. ^{1}H NMR ($CDCl_3$, 400.17 MHz, 300 K) spectrum of **Pt(L)Py**.

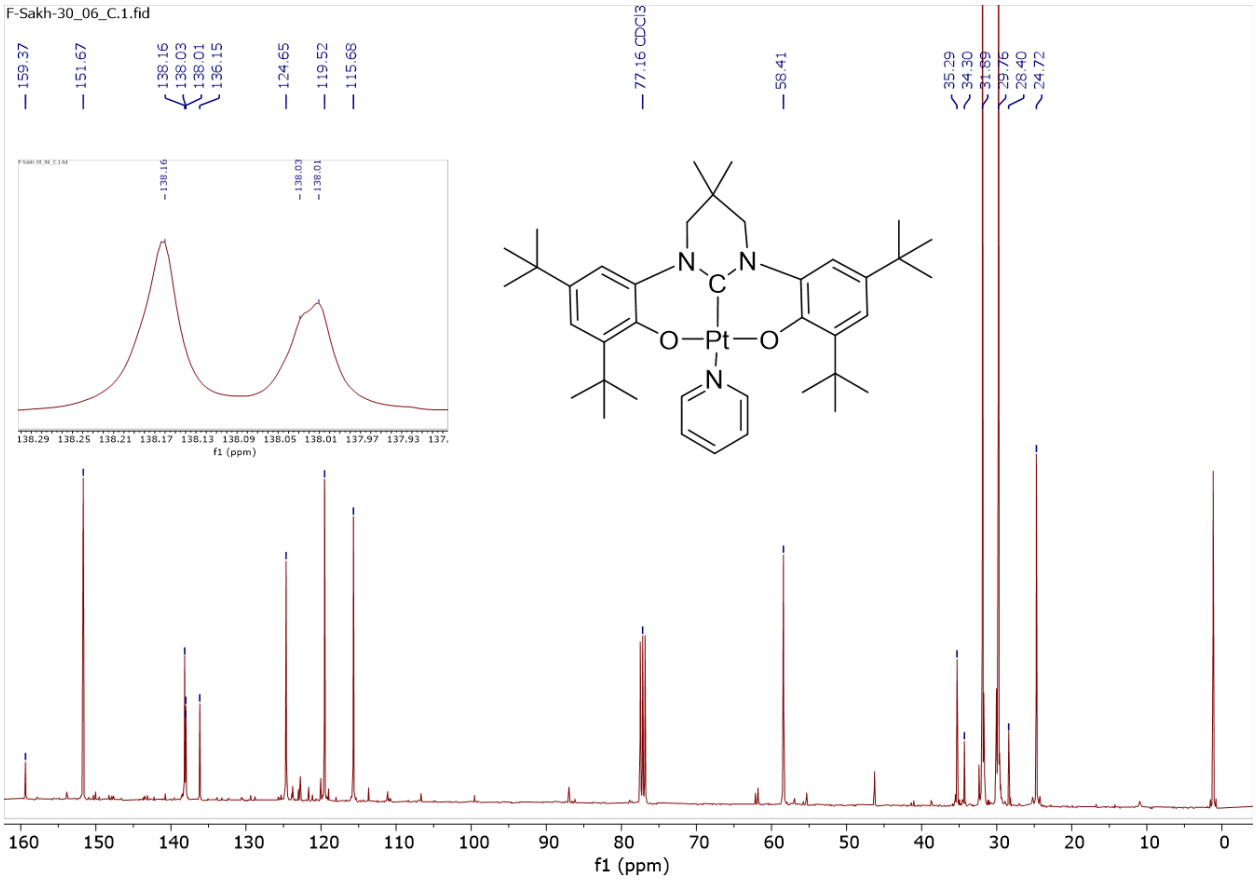


Figure S7. ^{13}C{^{1}H}NMR (100.62 MHz, $CDCl_3$, 300 K) spectrum of **Pt(L)Py**.