

Mechanism of electropolymerization of nickel(II) salen type complexes

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Supplementary materials:

Tab. S1. Comparison of FTIR ATR bands of *poly*[Ni(salcn)] films (electrosynthesized in Bu₄NPF₆ or Bu₄NClO₄) with FTIR bands of [Ni(salcn)] complex.

<i>complex</i>	<i>film</i>	<i>attributed to</i>	<i>comments</i>
1904(w)	-	overtones ⁴⁶	
1871(w)	-	overtones	
1832(w)	-	overtones	
	1750(vw)	overtones	
1624(s)	(s)	C=N ⁴⁴	
1601(s)	(m, sh)	CC aromatic ring ³⁶	
-	1562(m)	CC aromatic ring	
1541(s)	(m, sh)	CC aromatic ring	
1475(s)	(m, sh)	CC aromatic ring	
1454(s)	(m)	CH ₂ symmetric bending ⁴²	
1390(m)	(m)	C-N ⁴³	
1348(s)	(m)	C-H bending vibrations in cyclohexane moiety ⁴²	
1335(s)		C-H bending vibrations in cyclohexane moiety ⁴²	in films – overload with 1319
1319(s)	(m)	C-O stretching ⁴³	
1297(w)	(m)	Ar C-H in plane bends ^{36,37}	in film with PF ₆ ⁻ (m); in film with ClO ₄ ⁻ (w); moved to ~1292
-	1276(m, sh)	Ar C-H in plane bends and CH ₂ out of plane bendings in CH ₂ Cl ₂ ³⁶⁻³⁹	in film with PF ₆ ⁻ (m, sh); in film with ClO ₄ ⁻ (w, sh)
-	1247(m)	Ar C-H in plane bends ^{36,39}	
1227(w)		Ar C-H in plane bends	in film with PF ₆ ⁻ - overload with 1218; in film with ClO ₄ ⁻ - covered
-	1220-1000(s, br), max. 1092(s)	Cl-O ³⁵	absent in film with PF ₆ ⁻
-	1220-1000(s, br), max. 1079(s, sh)	Cl-O	absent in film with PF ₆ ⁻
1218(m)	(m, sh)	Ar C-H in plane bends ^{35,37}	in film with ClO ₄ ⁻ - covered by ClO ₄ ⁻ (1220-1000)
1192(m)	(w)	Ar C-H in plane bends	in film with PF ₆ ⁻ - moved to 1190 in film with ClO ₄ ⁻ - covered by ClO ₄ ⁻ (1220-1000)
-	1177(m, sh)	Ar C-H in plane bends	on band ClO ₄ ⁻ (m)
1142(s)	(m)	Ar C-H in plane bends	on band ClO ₄ ⁻ (m)
1121(m)	(w, sh)	Ar C-H in plane bends	in film with PF ₆ ⁻ - moved to 1125

			in film with ClO ₄ ⁻ - on band ClO ₄ ⁻ (m)
1109(w)	(w, sh)	Ar C-H in plane bends	in film with PF ₆ ⁻ - moved to 1104 in film with ClO ₄ ⁻ - covered by ClO ₄ ⁻ (1220-1000)
1043(m)	(w)	cyclohexane ring stretching and Ar C-H in plane bends ^{36,37,42}	covered by ClO ₄ ⁻ (1220-1000)
1009(m)	(w)	cyclohexane ring stretching and Ar C-H in plane bends	in film with PF ₆ ⁻ - moved to 1014 in film with ClO ₄ ⁻ - covered by ClO ₄ ⁻ (1220-1000)
-	1000(w, sh)	Cl-O ³⁵	absent in film with PF ₆ ⁻
-	978(w)	Ar C-H in plane bends ^{36,37}	
947(m)	(w, sh)	Ar C-H in plane bends	in films - moved to 943
912(w)	-		in films - overload with 908
908(s)	(w)	cyclohexane, ring stretching ⁴²	in film with PF ₆ ⁻ - (w); in film with ClO ₄ ⁻ - (m)
-	892(m)	Ar C-H out of plane bending and CH ₂ Cl ₂ ³⁶⁻³⁹	covered by PF ₆ ⁻ (900-800);
-	874(w, sh)	Ar C-H out of plane bending ^{36,37}	covered by PF ₆ ⁻ (900-800);
-	900-800 (s, br), max. 844(s)	P-F ³⁴	absent in film with ClO ₄ ⁻
846(s)	(w)	cyclohexane, ring stretching ⁴²	in film with ClO ₄ ⁻ - moved to 852 in film with PF ₆ ⁻ - covered by PF ₆ ⁻ (900-800)
-	818(w)	Ar C-H out of plane bending ^{36,37}	covered by PF ₆ ⁻ (900-800)
-	804(w)	Ar C-H out of plane bending	covered by PF ₆ ⁻ (900-800);
798(w)	(w, sh)		
-	780-600(m, br), max. 702(m)	Cl-O ³⁵	absent in film with PF ₆ ⁻
750(s)	(w)	Ar C-H out of plane bending and C-Cl stretching ³⁶⁻³⁹	on band ClO ₄ ⁻ (780 -600)
738(s)	(w)	Ar C-H out of plane bending ³⁶⁻³⁹	on band ClO ₄ ⁻ (780 -600)
-	703(w, sh)	Ar C-H out of plane bending and C-Cl stretching	covered by ClO ₄ ⁻ (780 -600)
689(w)	(w, sh)	Ar CC out of plane bending	in film with PF ₆ ⁻ - moved to 682 in film with ClO ₄ ⁻ - on band ClO ₄ ⁻ (780 -600)
681(w)	(w, sh)	Ar CC out of plane bending	in film with PF ₆ ⁻ - moved to 677 in film with ClO ₄ ⁻ - on band ClO ₄ ⁻ (780 -600)
618(w)	(w)	Ni-N	absent on ligand spectrum
581(s)	(m)	Ni-O	absent on ligand spectrum
-	568(m)	P-F ³⁴	absent in film with ClO ₄ ⁻
547(w)	(w)		in film with PF ₆ ⁻ - (w); in film with ClO ₄ ⁻ - (m)

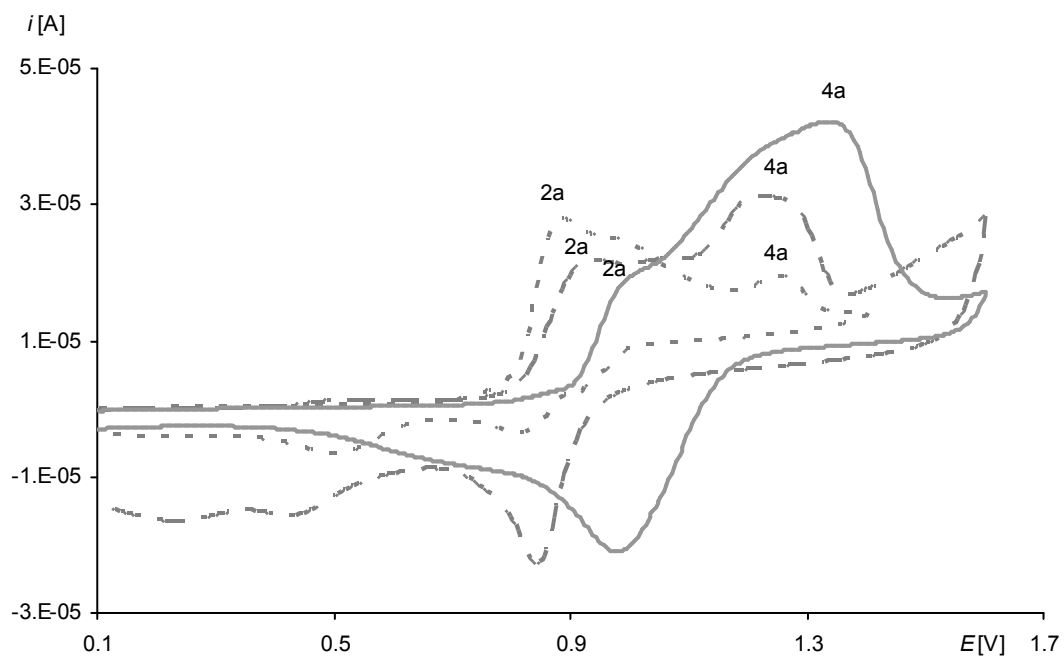


Fig.S1 Cyclic voltammograms of complexes in TBAH/CH₂Cl₂, 0.1÷1.6 V, $\nu = 0.05 \text{ V}\cdot\text{s}^{-1}$, 1st scans vs. Ag/AgCl; T=293K; solid line – [Ni(salcn)], dashed line – [Ni(salcn(Me))], dotted line - [Ni(salcn(Bu))].

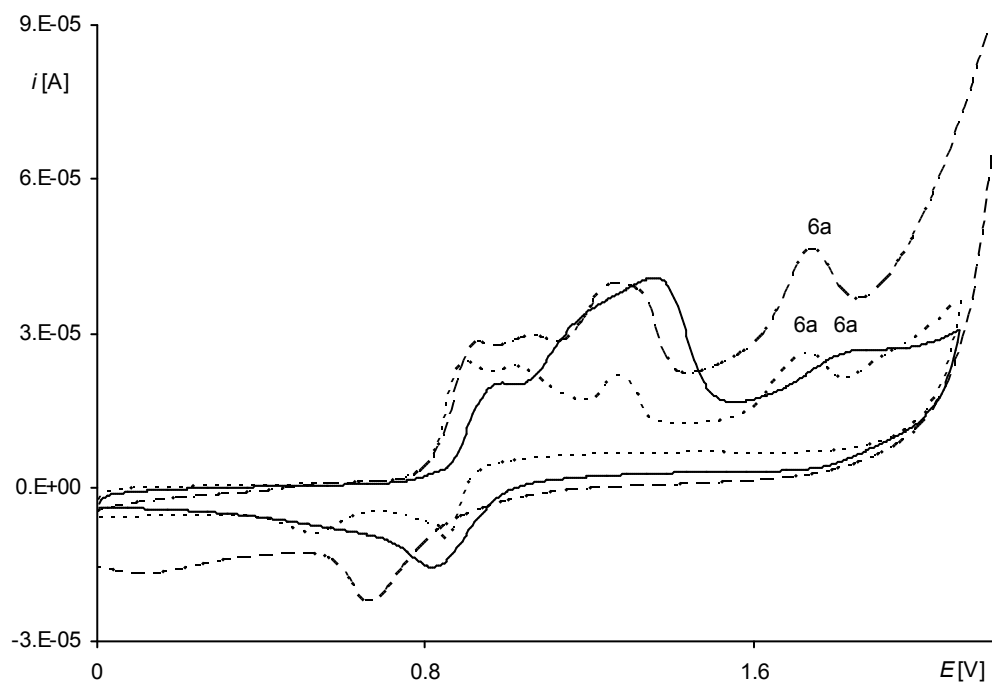


Fig.S2 Cyclic voltammograms of complexes in TBAH/CH₂Cl₂, 0.1÷2.1 V, $\nu = 0.05 \text{ V}\cdot\text{s}^{-1}$, 1st scans vs. Ag/AgCl; T=293K; solid line – [Ni(salcn)], dashed line – [Ni(salcn(Me))], dotted line - [Ni(salcn(Bu))].