

Shift of Redox Potential of Nickel(II) Schiff Base Complexes in Presence of Redox Innocent Metal Ions

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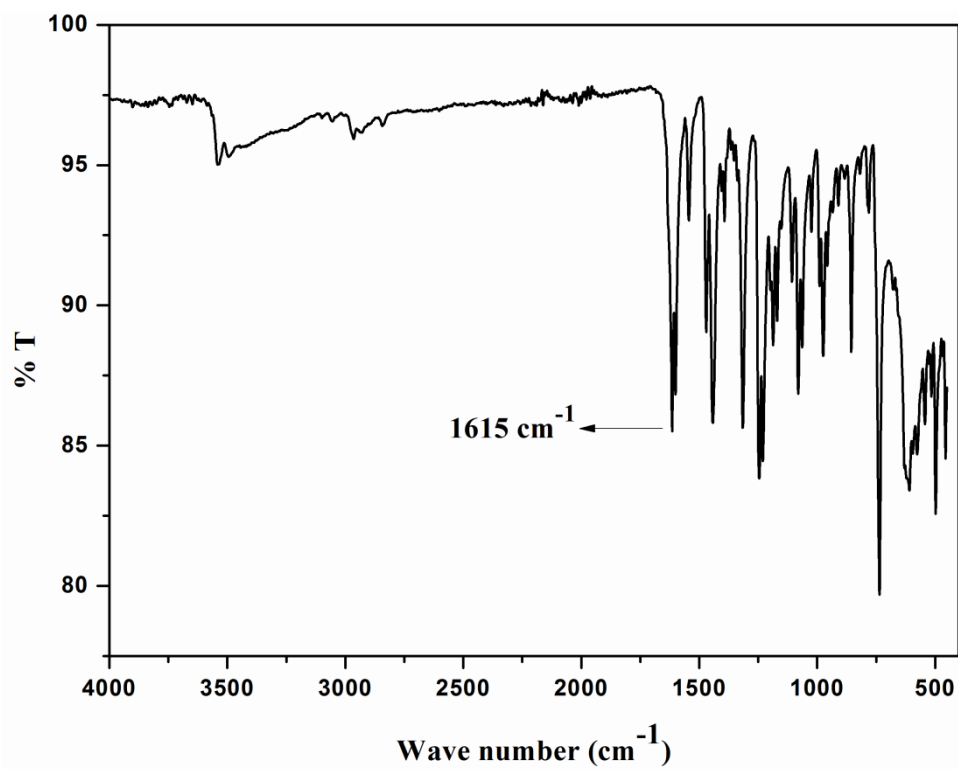


Fig. S1 IR spectrum of NiL^{en}.

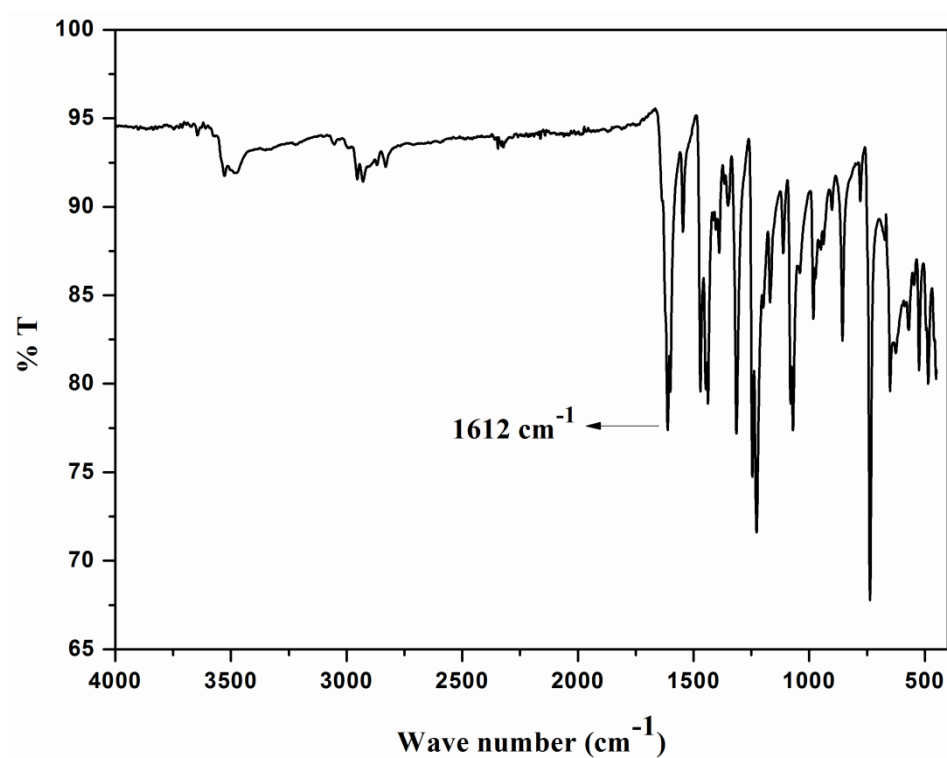


Fig. S2 IR spectrum of NiL^{pn}.

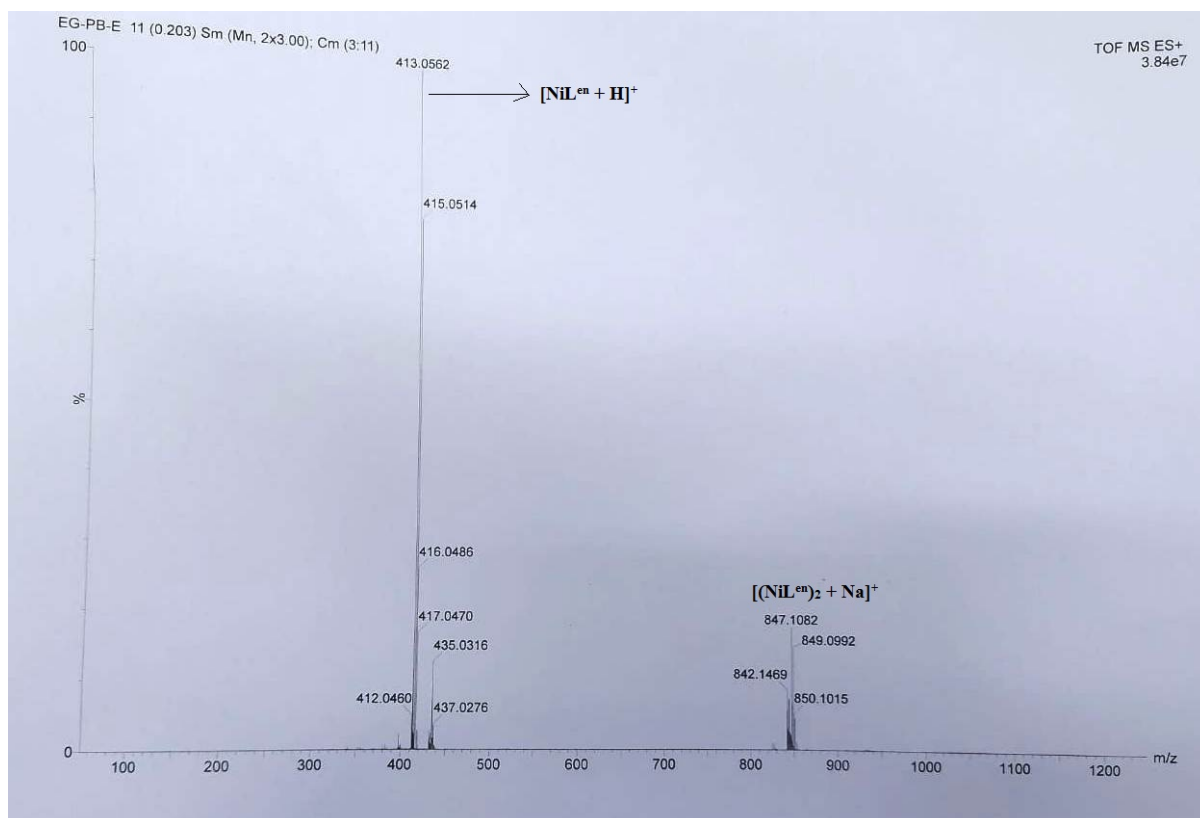


Fig. S3 Mass spectrometric analysis of NiL^{en} .

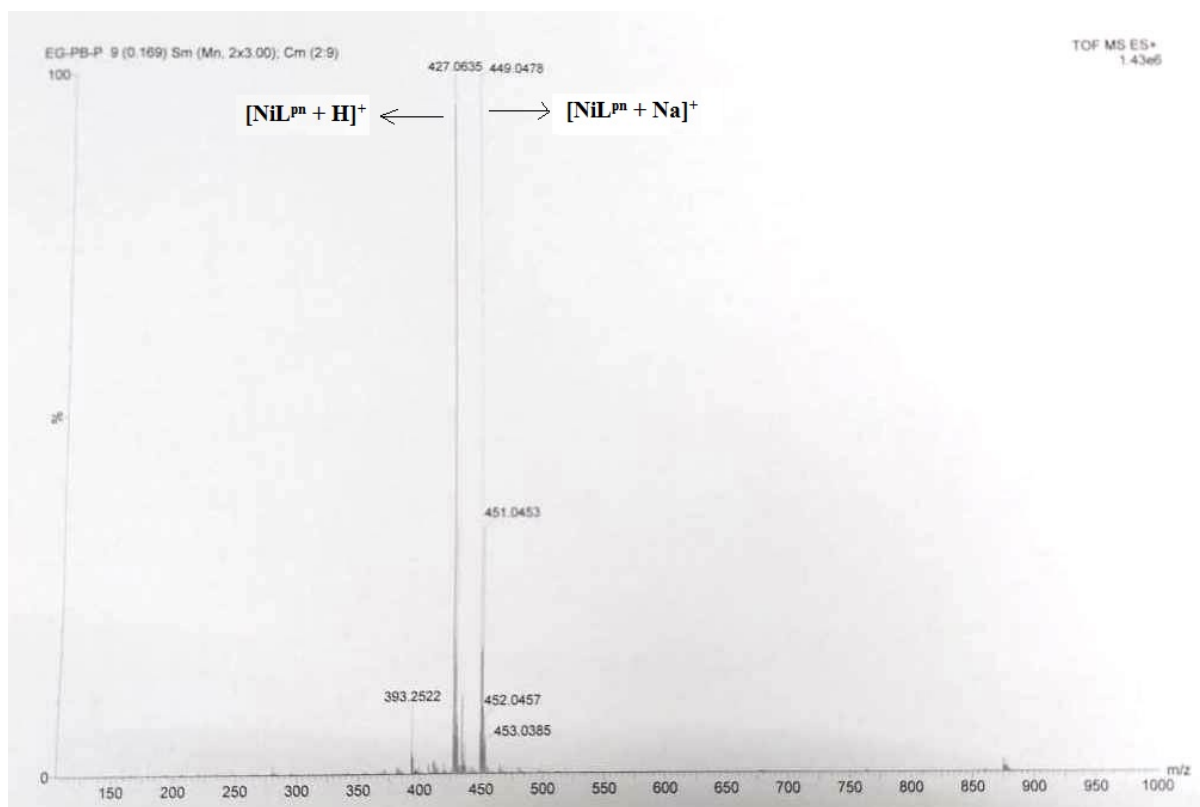


Fig. S4 Mass spectrometric analysis of NiL^{pn} .

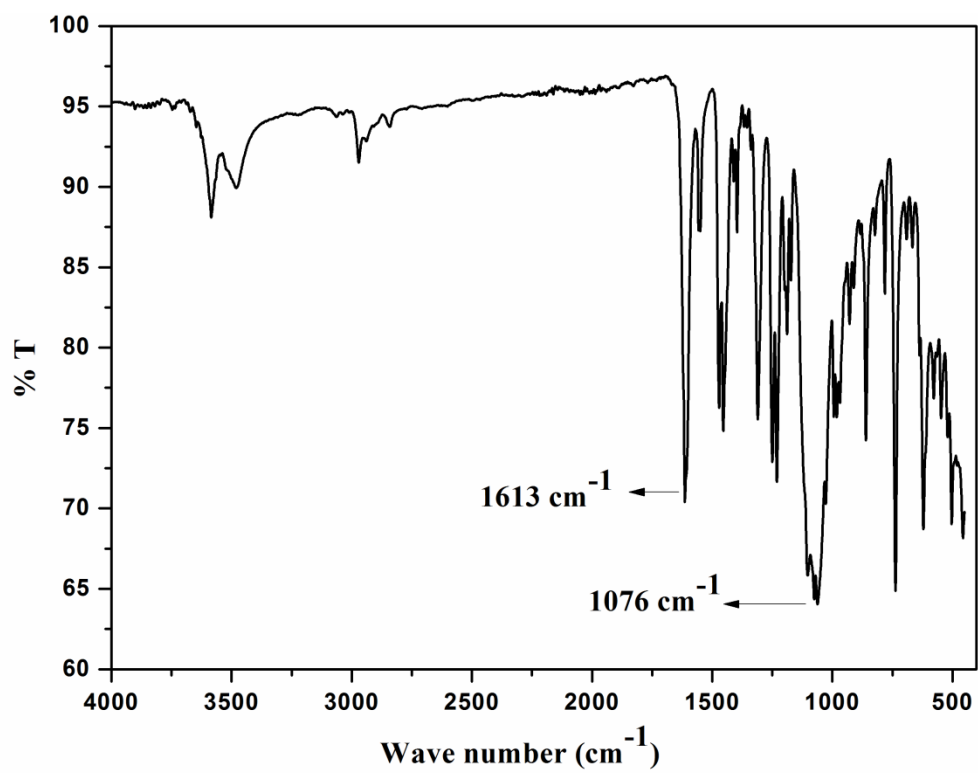


Fig. S5 IR spectrum of complex 1.

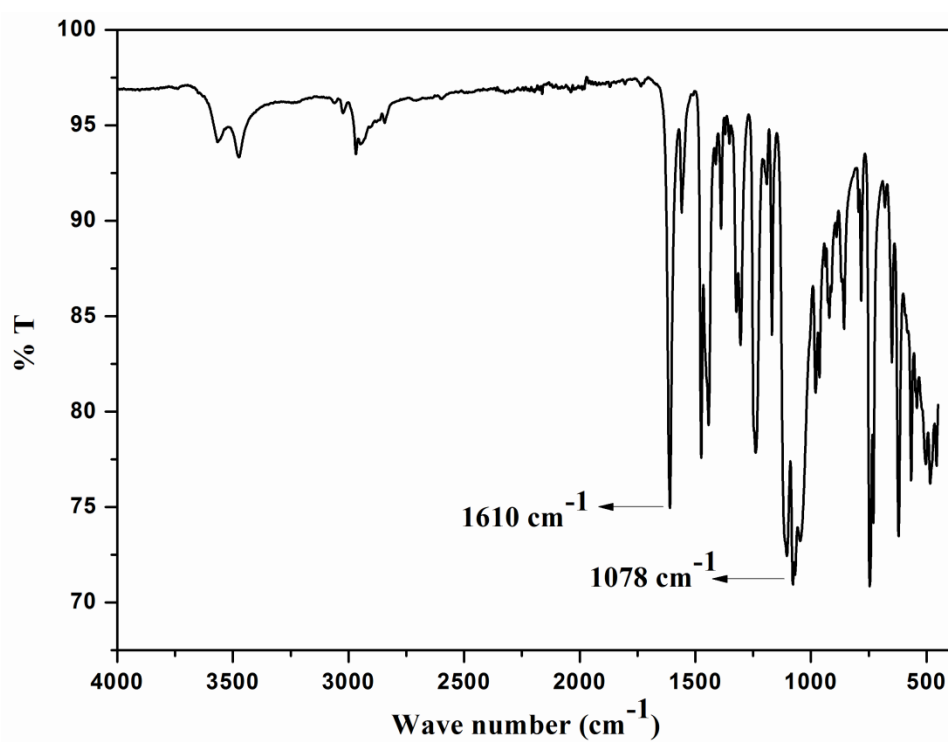


Fig. S6 IR spectrum of complex 2.

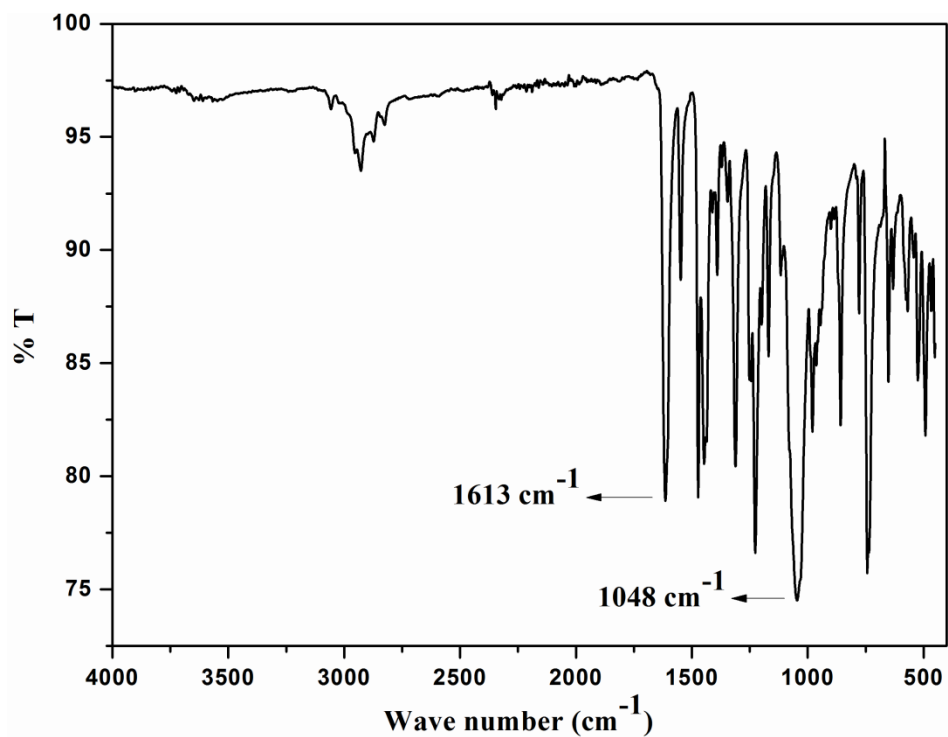


Fig. S7 IR spectrum of complex 3.

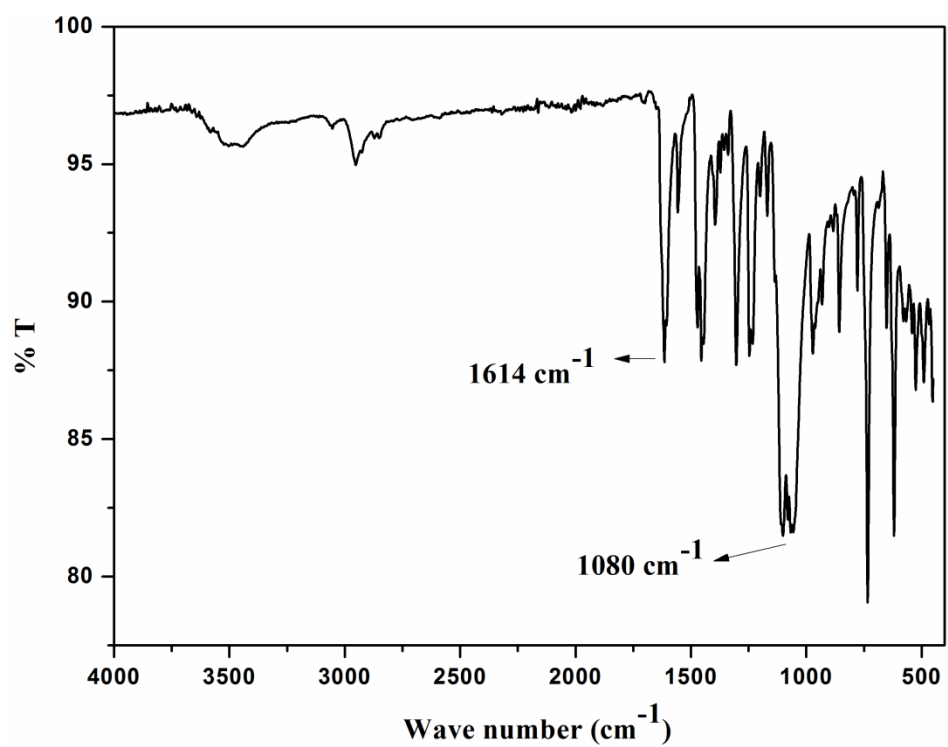


Fig. S8 IR spectrum of complex 4.

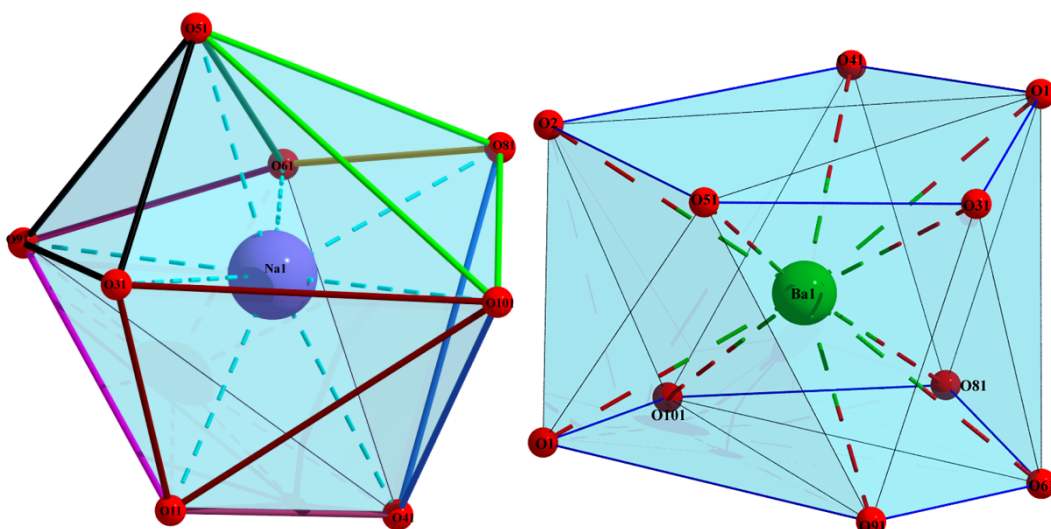


Fig. S9 Polyhedral view of the coordination sphere around the sodium and barium centres for complexes **3** (left) and **4** (right), respectively.

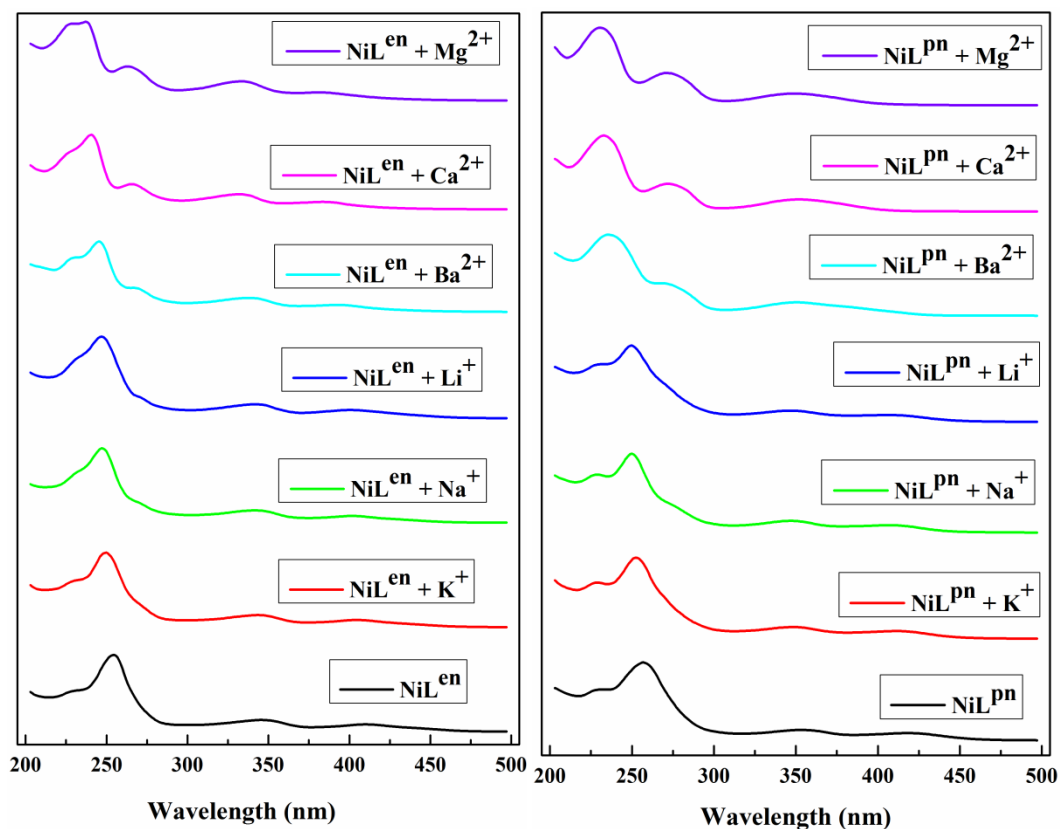


Fig. S10 CT spectra of 5×10^{-5} M nickel complexes, $[\text{NiL}^{\text{en}}]$ (left) and $[\text{NiL}^{\text{pn}}]$ (right) in presence of equivalent amount of each of Li^+ , Na^+ , K^+ , Mg^{2+} , Ca^{2+} and Ba^{2+} ions in acetonitrile solution.

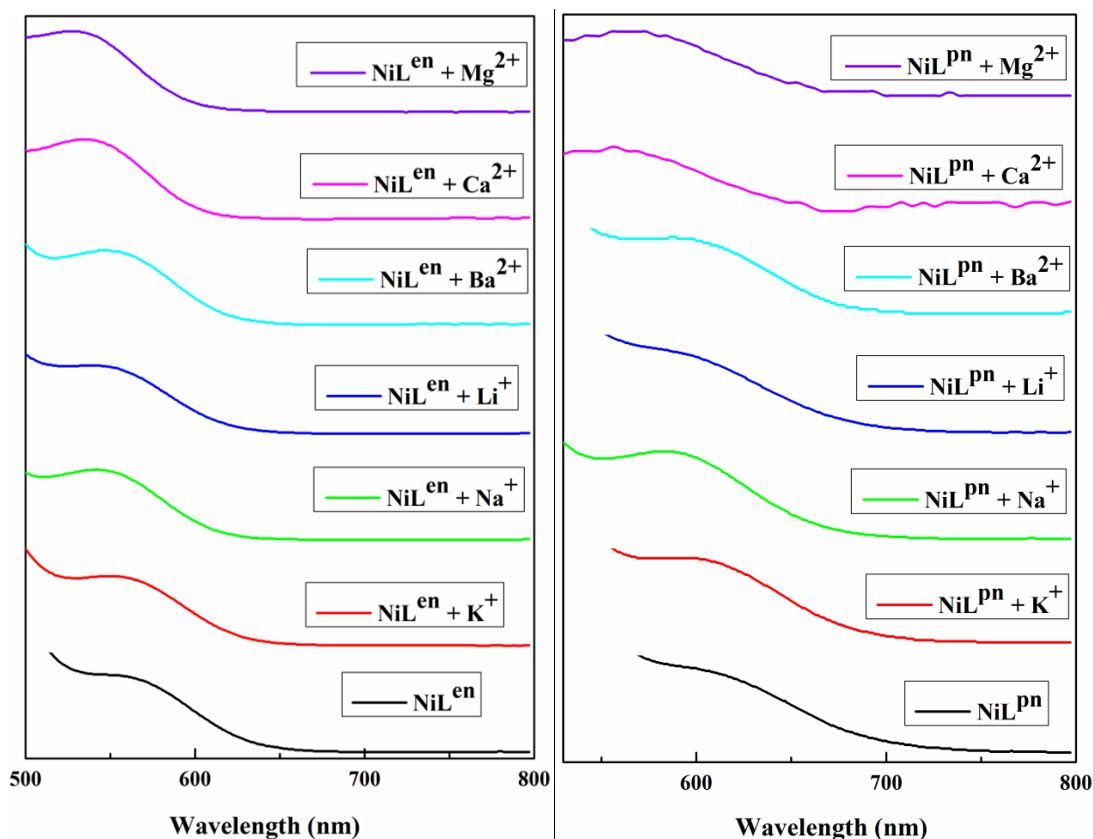


Fig. S11 d-d spectra of 10^{-3} M nickel complexes, $[\text{NiL}^{\text{en}}]$ (left) and $[\text{NiL}^{\text{pn}}]$ (right) in presence of equivalent amount of each of Li^+ , Na^+ , K^+ , Mg^{2+} , Ca^{2+} and Ba^{2+} ions in acetonitrile solution.

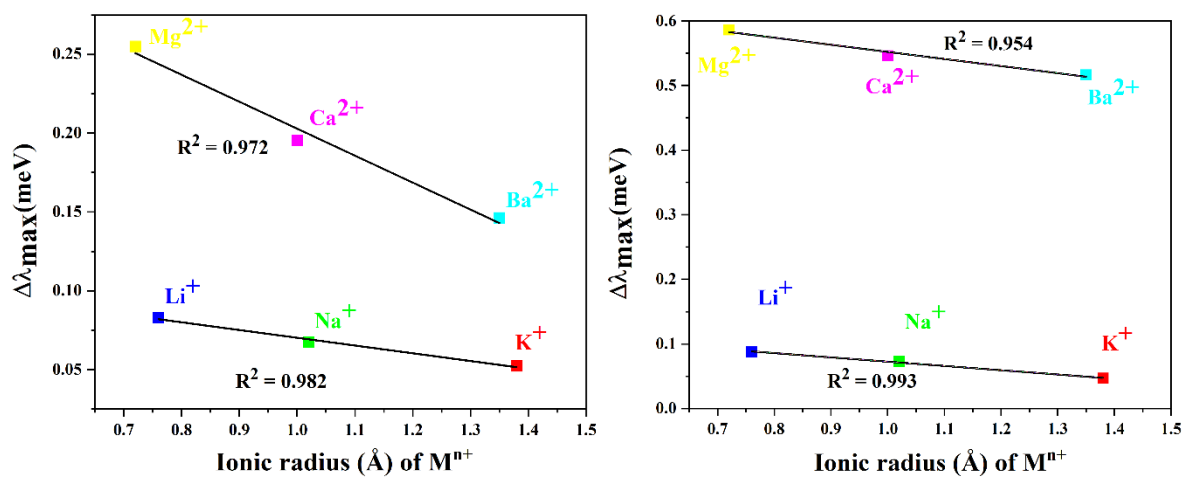


Fig. S12 Dependence of MLCT energy of Lewis acid bound nickel metalloligands on the ionic radius of the corresponding metal ions (left, $[\text{NiL}^{\text{en}}]$) and (right, $[\text{NiL}^{\text{pn}}]$).

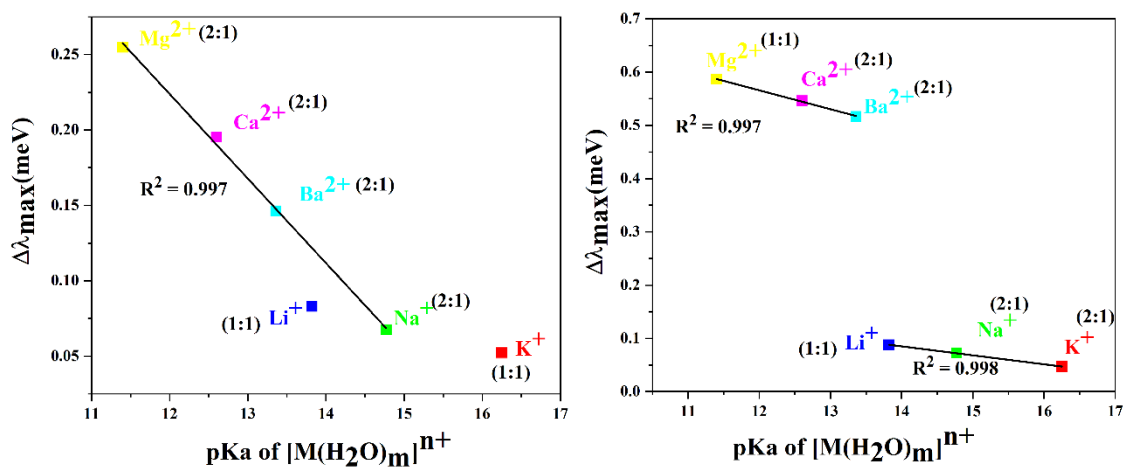


Fig. S13 Dependence of MLCT energy of Lewis acid bound nickel metalloligands on the pKa value of the corresponding metal ions (left, $[\text{NiL}^{\text{en}}]$) and (right, $[\text{NiL}^{\text{pn}}]$).

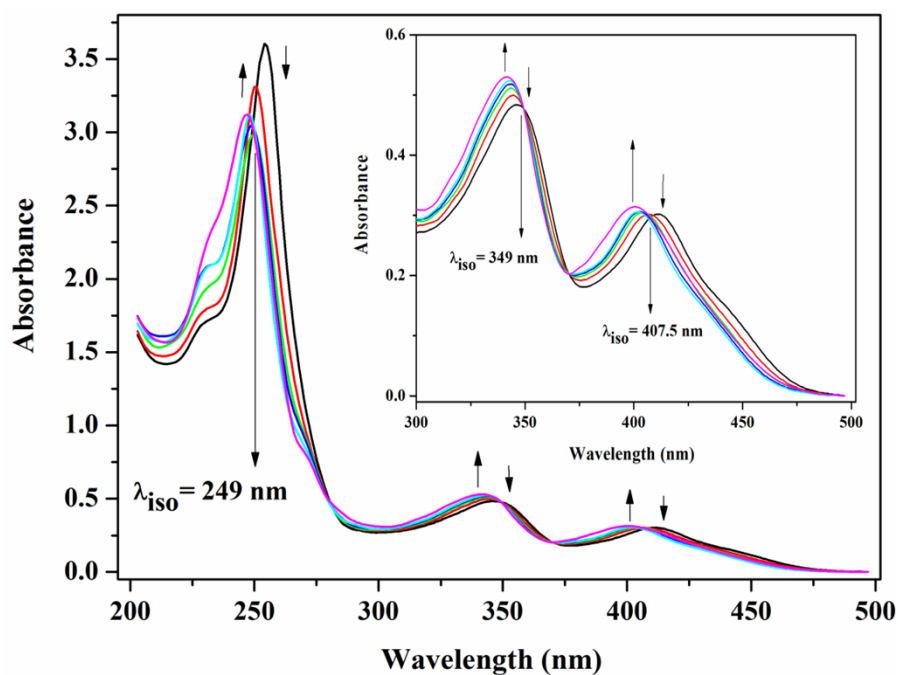


Fig. S14 Spectrophotometric titration of 5×10^{-5} M acetonitrile solution of $[\text{NiL}^{\text{en}}]$ by LiClO_4 .

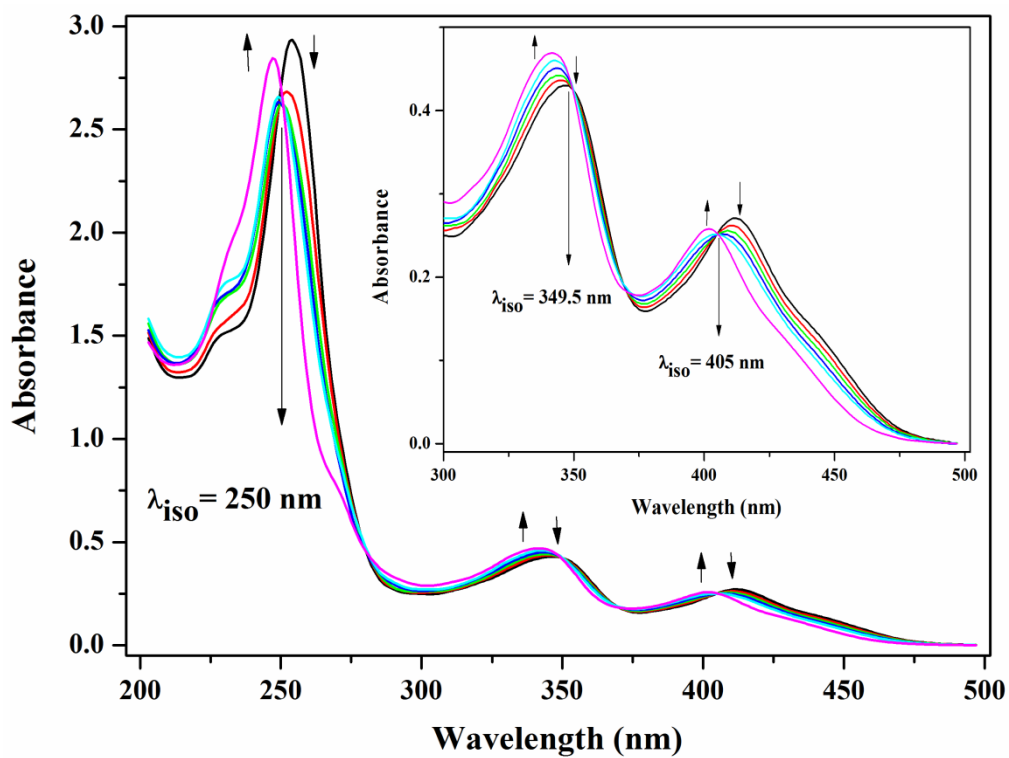


Fig. S15 Spectrophotometric titration of 5×10^{-5} M acetonitrile solution of $[\text{NiL}^{\text{en}}]$ by NaBF_4 .

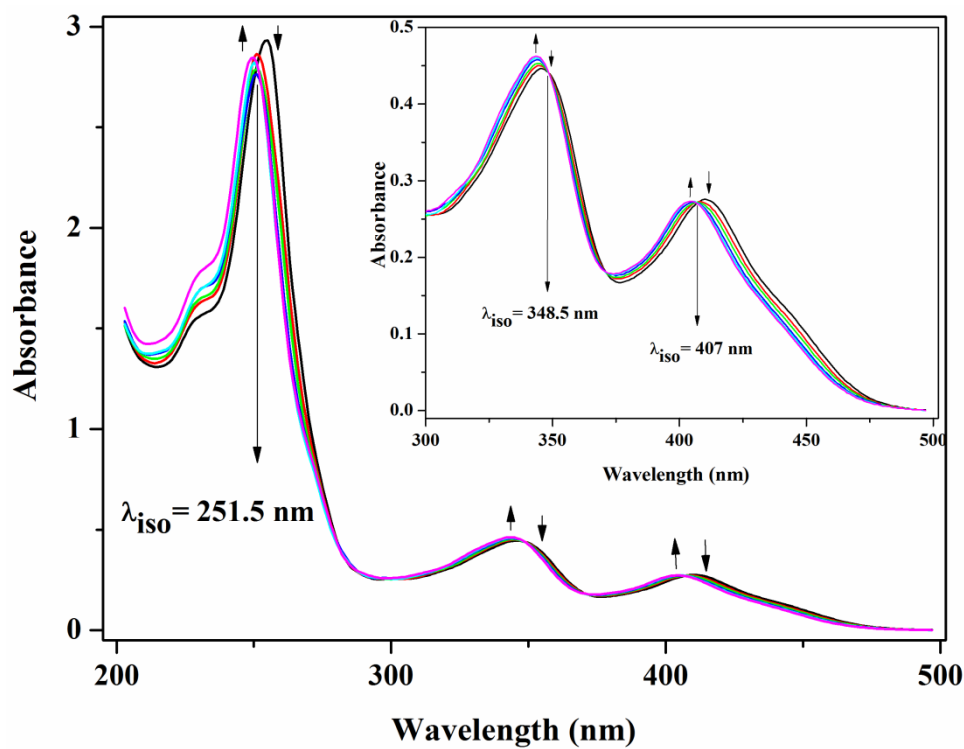


Fig. S16 Spectrophotometric titration of 5×10^{-5} M acetonitrile solution of $[\text{NiL}^{\text{en}}]$ by KPF_6 .

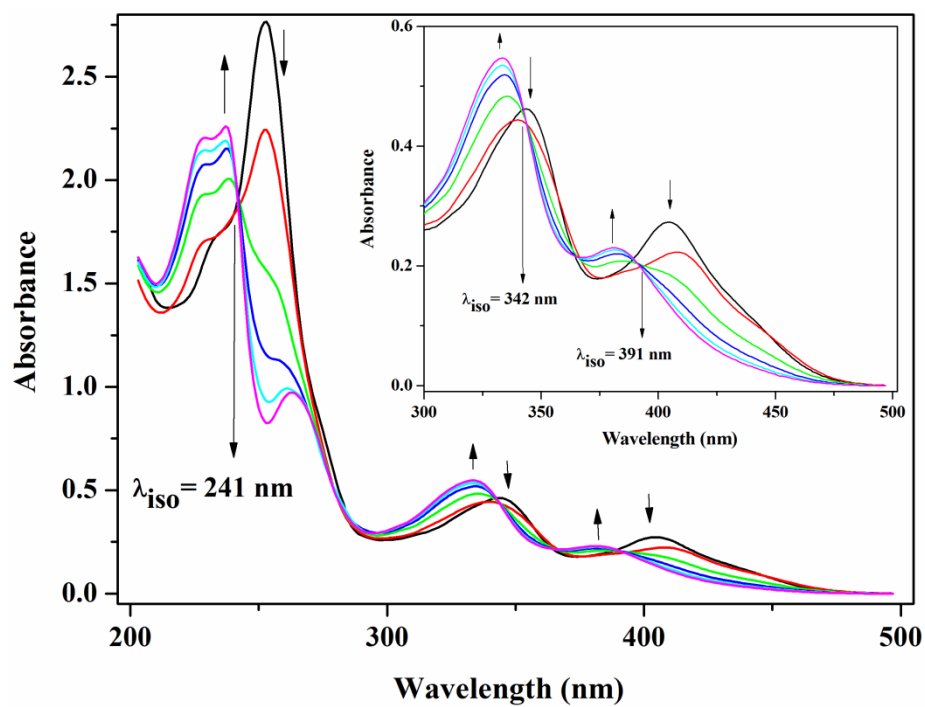


Fig. S17 Spectrophotometric titration of 5×10^{-5} M acetonitrile solution of $[\text{NiL}^{\text{en}}]$ by $\text{Mg}(\text{ClO}_4)_2$.

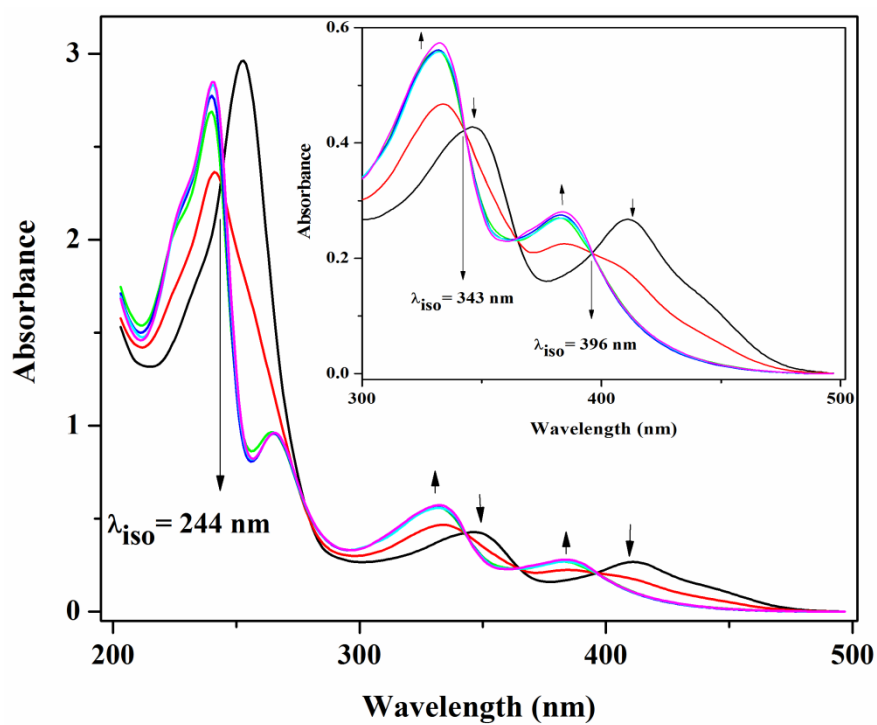


Fig. S18 Spectrophotometric titration of 5×10^{-5} M acetonitrile solution of $[\text{NiL}^{\text{en}}]$ by $\text{Ca}(\text{ClO}_4)_2$.

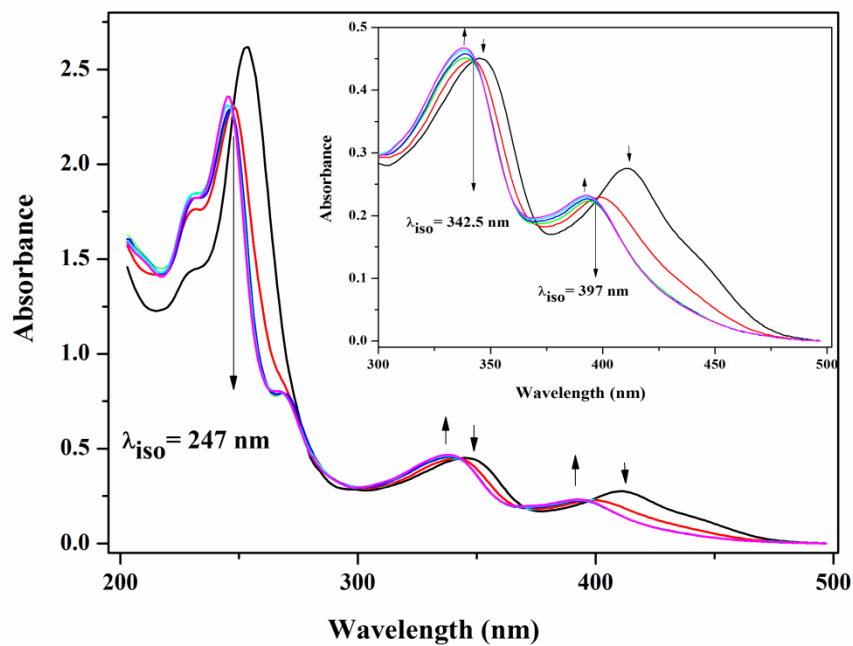


Fig. S19 Spectrophotometric titration of $5 \times 10^{-5} \text{ M}$ acetonitrile solution of $[\text{NiL}^{\text{en}}]$ by $\text{Ba}(\text{ClO}_4)_2$.

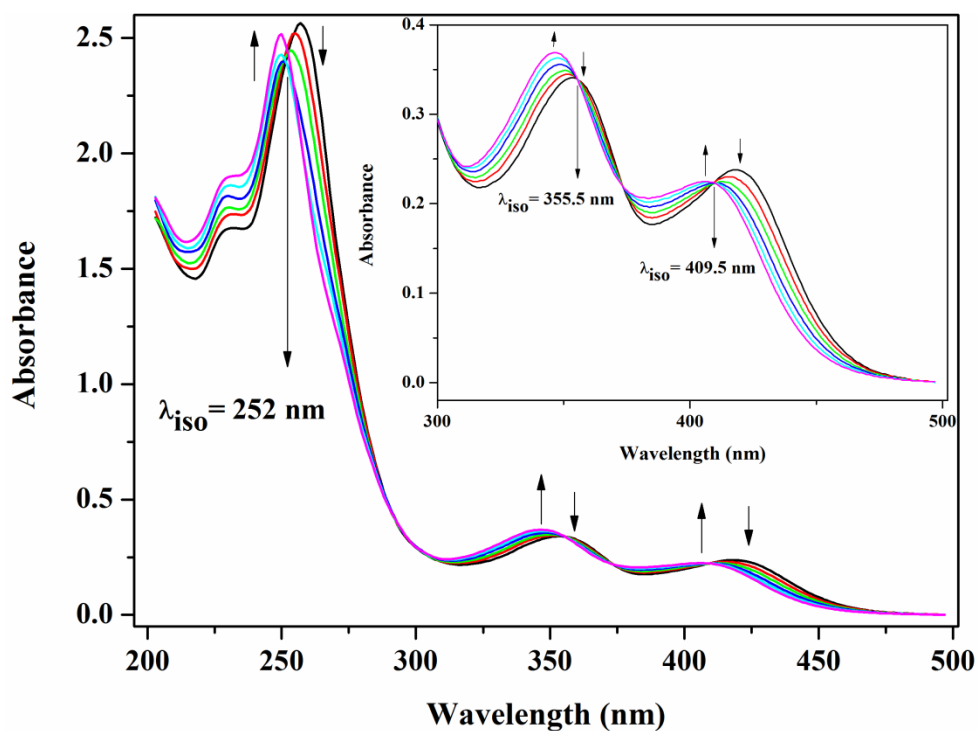


Fig. S20 Spectrophotometric titration of $5 \times 10^{-5} \text{ M}$ acetonitrile solution of $[\text{NiL}^{\text{pn}}]$ by LiClO_4 .

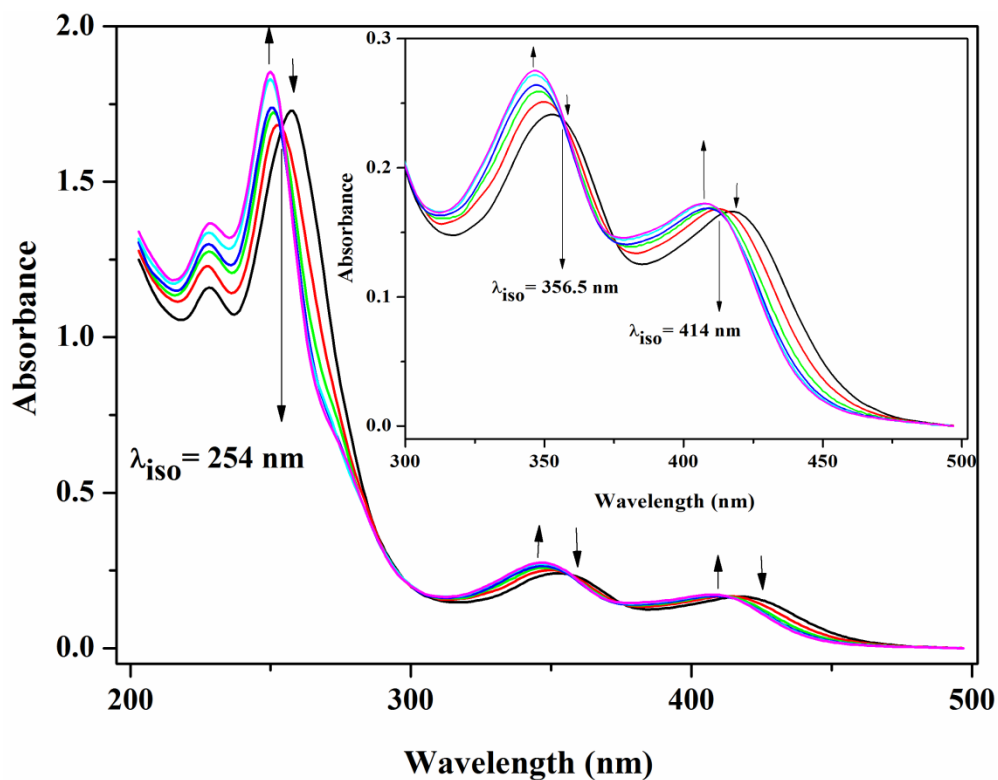


Fig. S21 Spectrophotometric titration of 5×10^{-5} M acetonitrile solution of $[\text{NiL}^{\text{pn}}]$ by NaBF_4 .

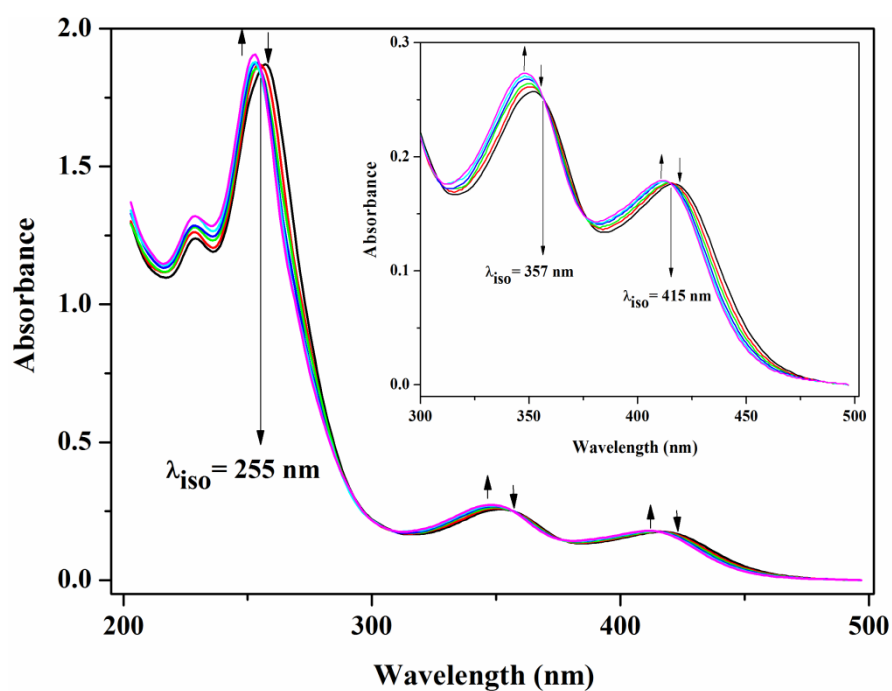


Fig. S22 Spectrophotometric titration of 5×10^{-5} M acetonitrile solution of $[\text{NiL}^{\text{pn}}]$ by KPF_6 .

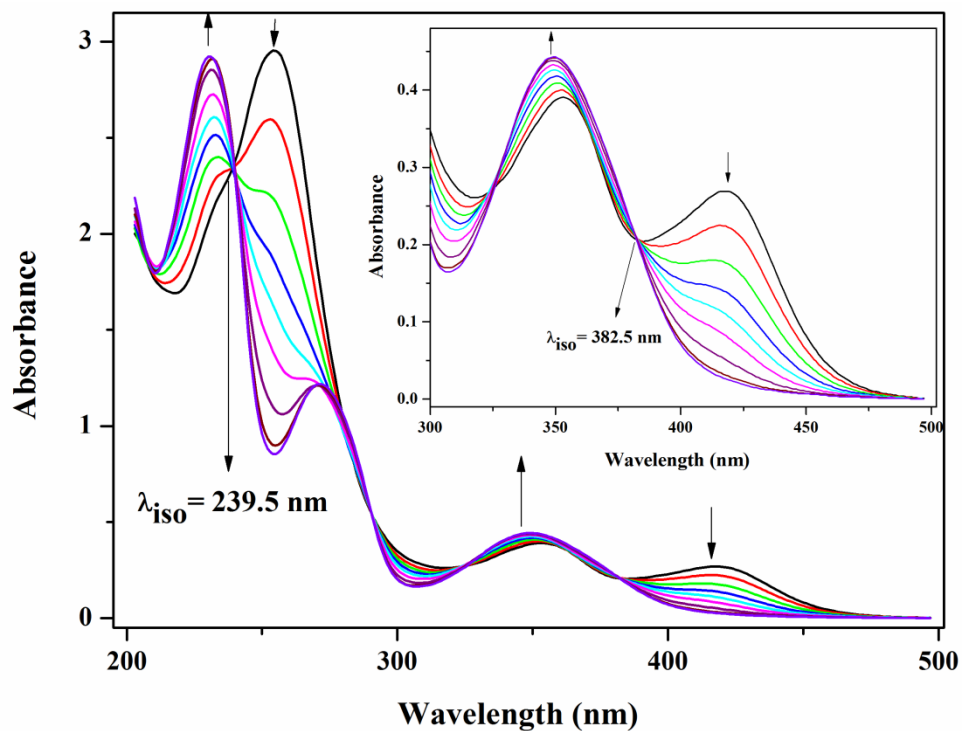


Fig. S23 Spectrophotometric titration of 5×10^{-5} M acetonitrile solution of $[\text{NiL}^{\text{Pn}}]$ by $\text{Mg}(\text{ClO}_4)_2$.

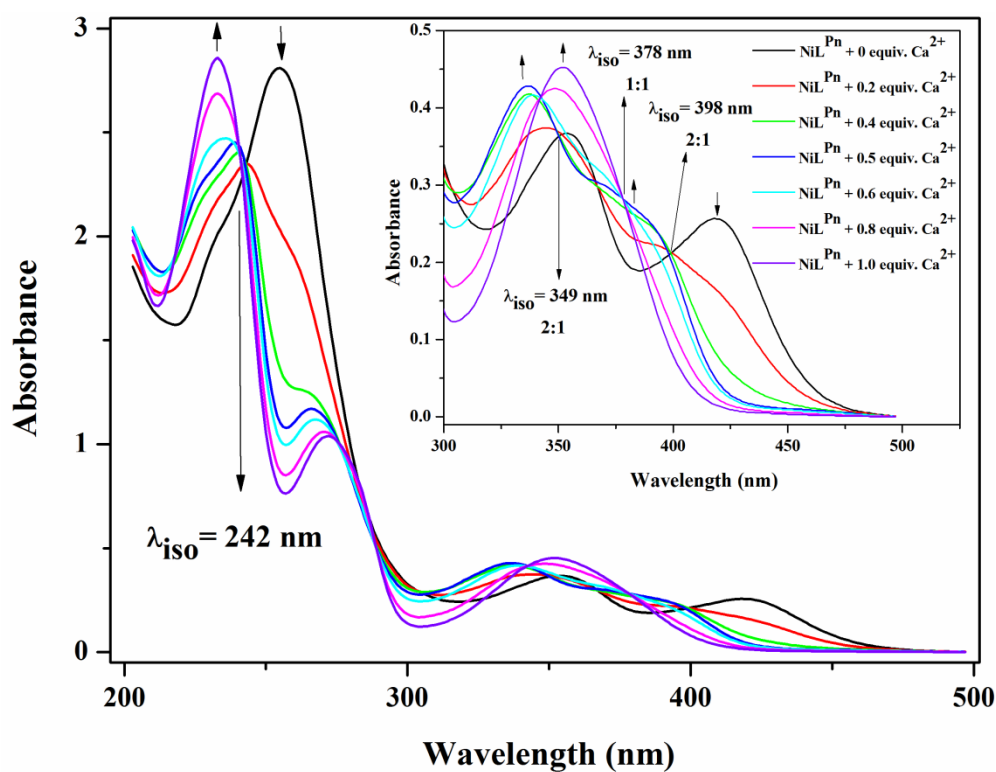


Fig. S24 Spectrophotometric titration of 5×10^{-5} M acetonitrile solution of $[\text{NiL}^{\text{Pn}}]$ by $\text{Ca}(\text{ClO}_4)_2$.

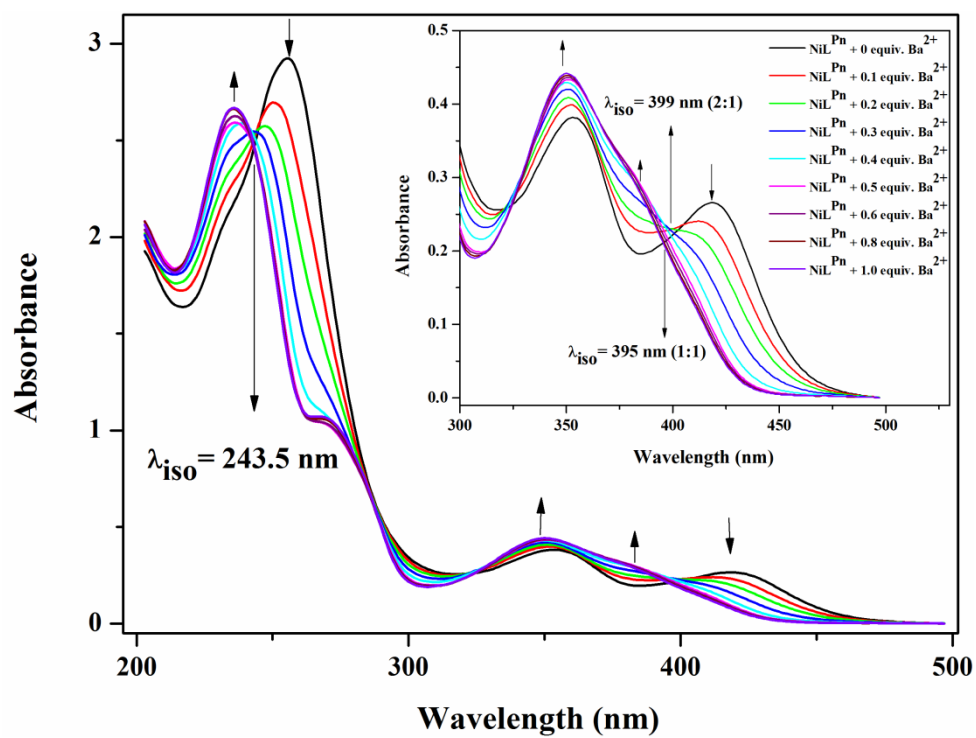


Fig. S25 Spectrophotometric titration of 5×10^{-5} M acetonitrile solution of $[\text{NiL}^{\text{Pn}}]$ by $\text{Ba}(\text{ClO}_4)_2$.

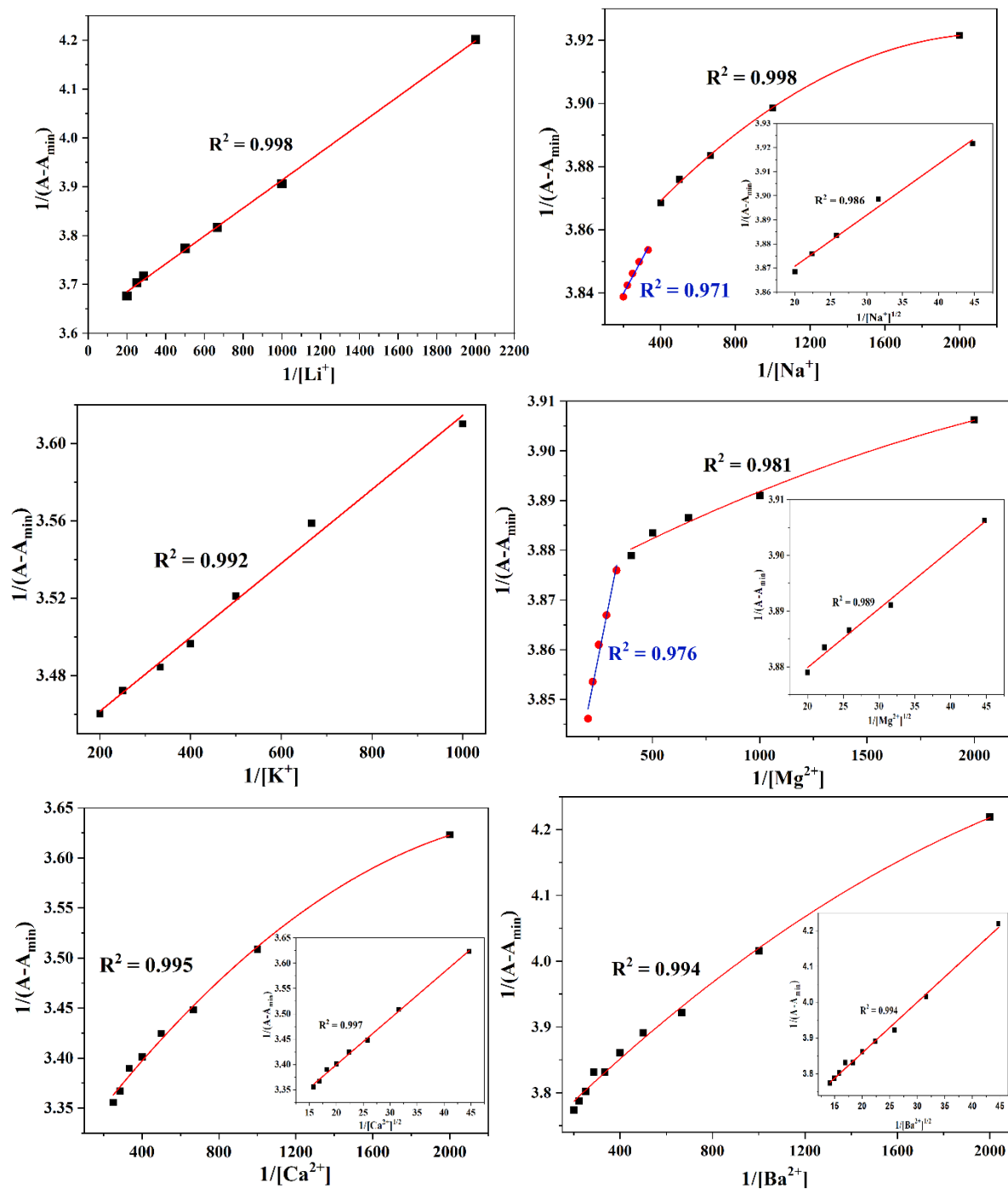


Fig. S26 Benesi–Hildebrand plot for the associative interaction of $[NiL^{en}]$ complex with respective metal ions in acetonitrile. Insert shows the inverse of absolute change in absorbance vs. the inverse of square root of metal ions concentration for the 2 : 1 ($[NiL^{en}] : M^{n+}$) cases.

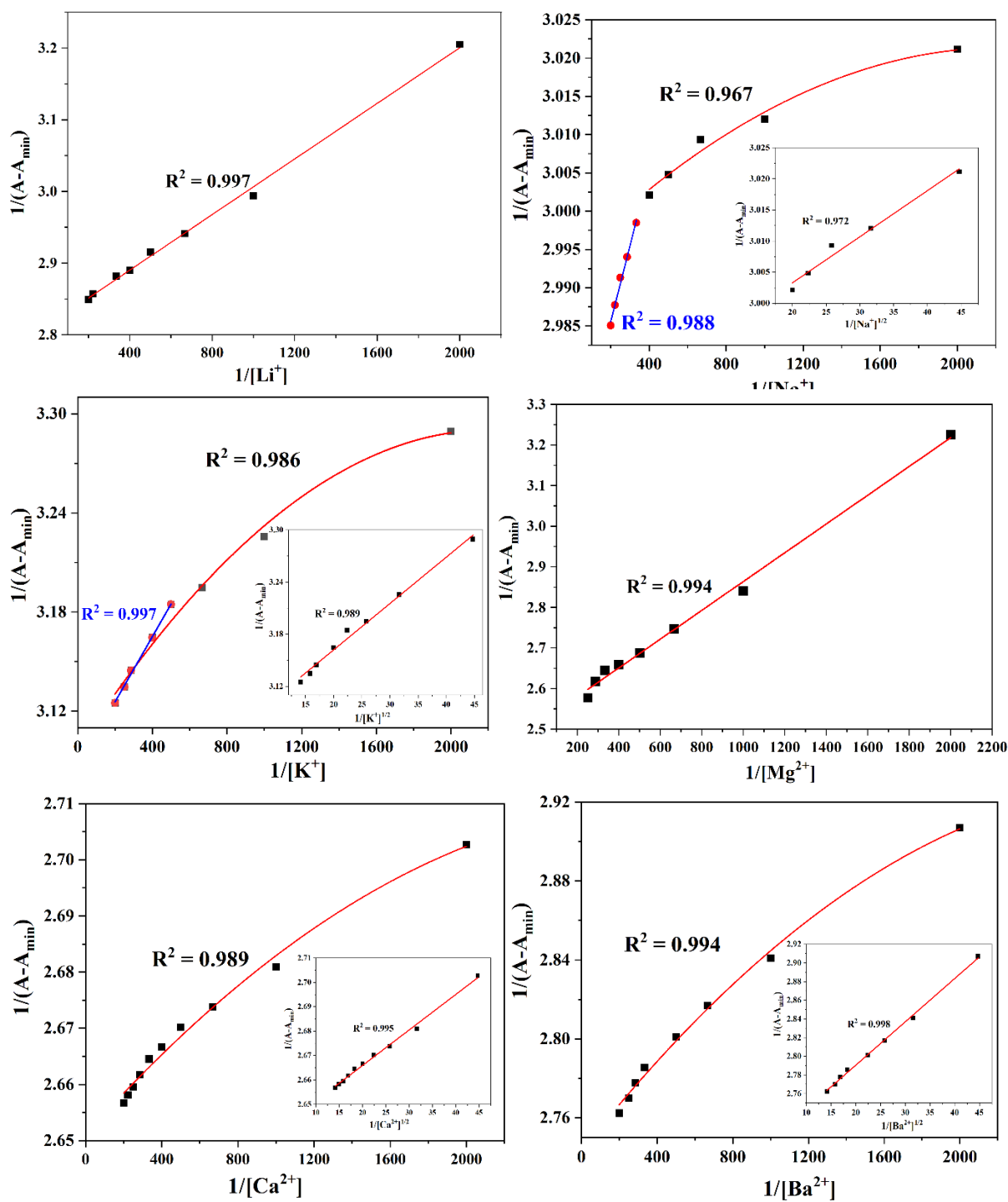


Fig. S27 Benesi–Hildebrand plot for the associative interaction of $[NiL^{pn}]$ complex with respective metal ions in acetonitrile. Insert shows the inverse of absolute change in absorbance vs. the inverse of square root of metal ions concentration for the 2 : 1 ($[NiL^{pn}] : M^{n+}$) cases.

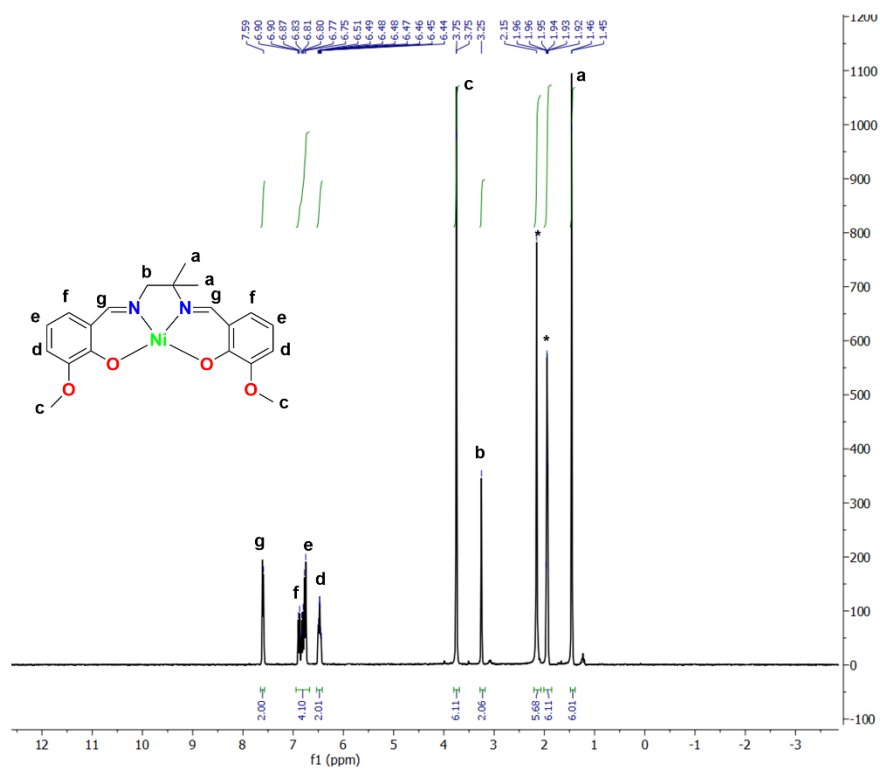


Fig. S28 $^1\text{H-NMR}$ spectrum of NiL^{en} in CD_3CN .

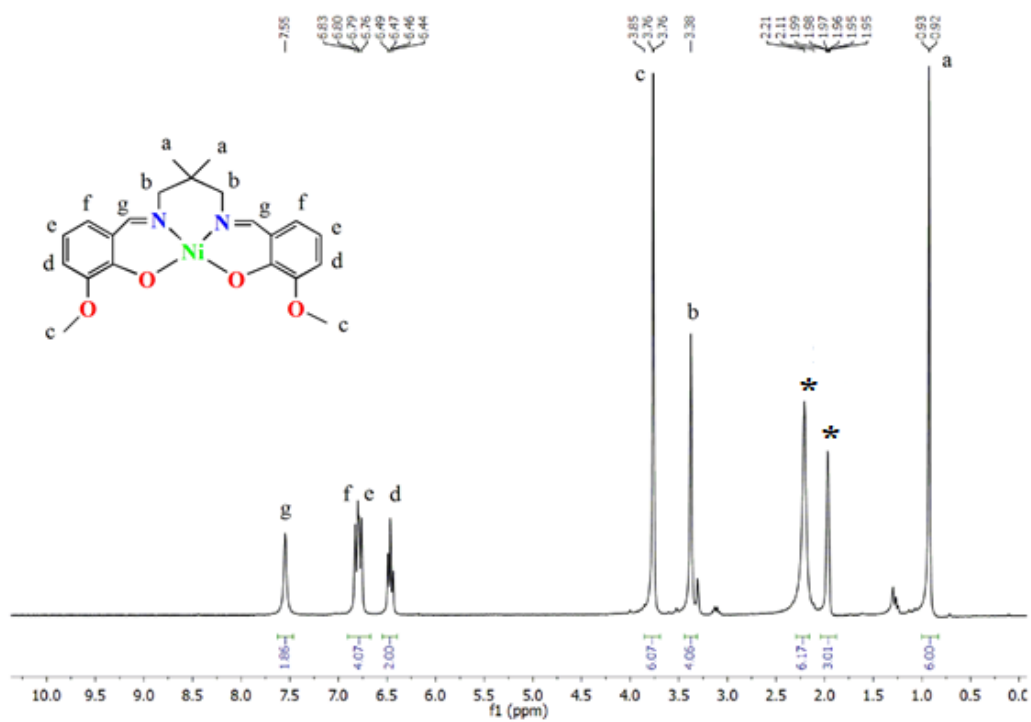


Fig. S29 $^1\text{H-NMR}$ spectrum of NiL^{pn} in CD_3CN .

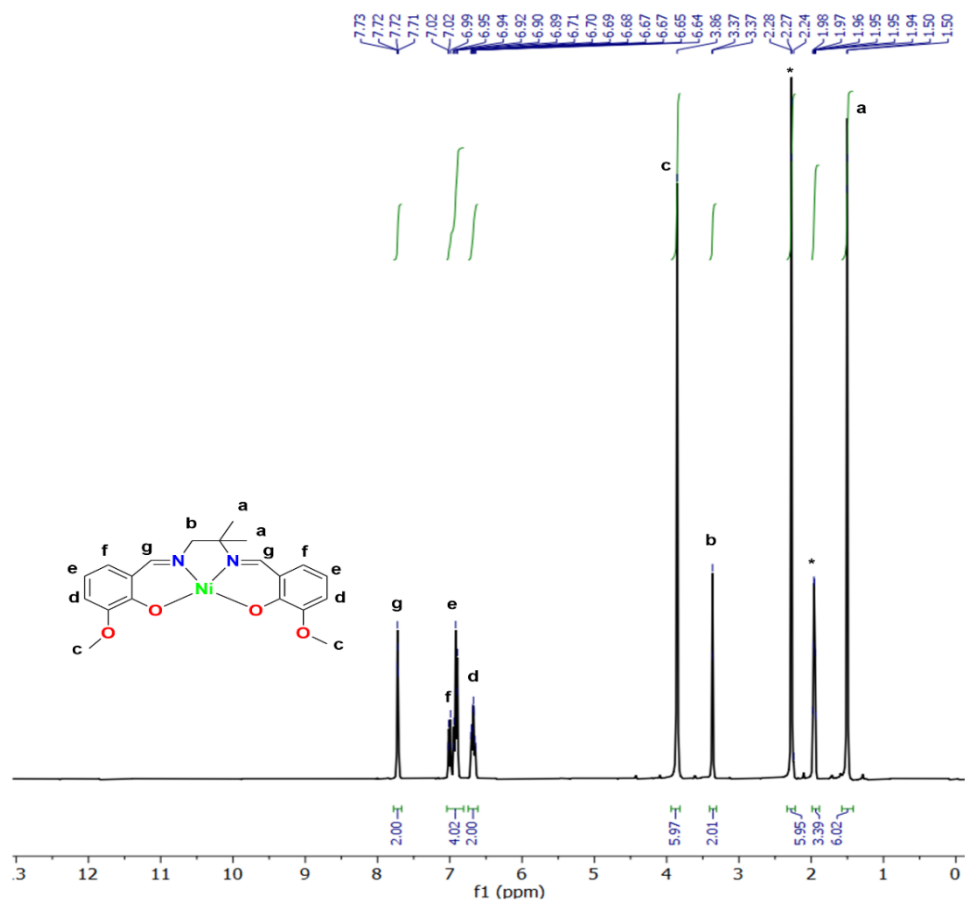


Fig. S30 ¹H-NMR spectrum of NiLⁿ in presence of LiClO₄ in CD₃CN.

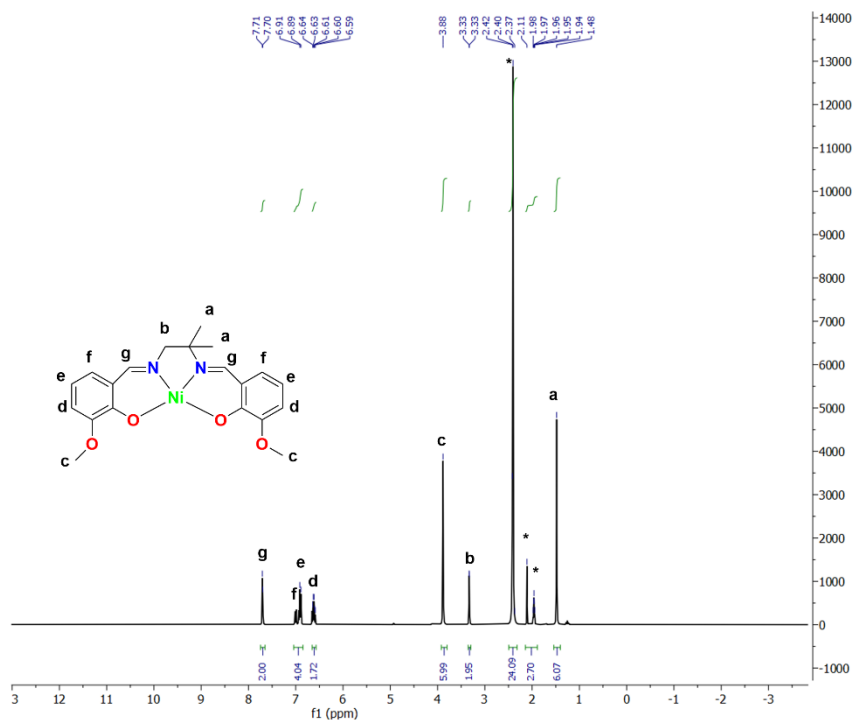


Fig. S31 ¹H-NMR spectrum of NiLⁿ in presence of NaBF₄ in CD₃CN.

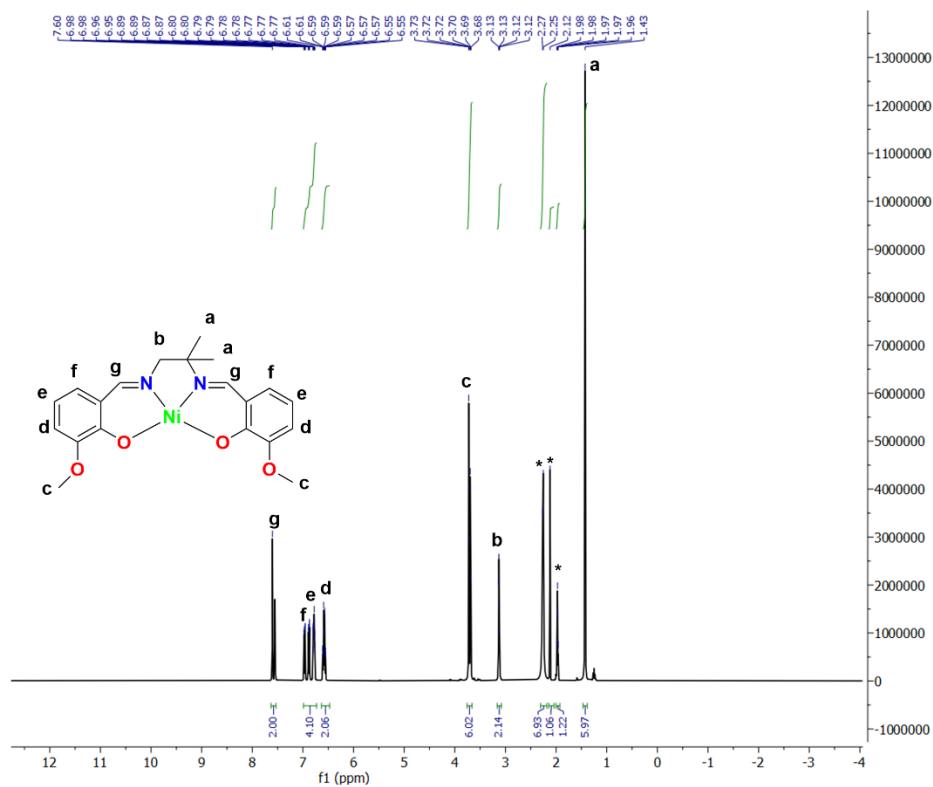


Fig. S32 1H -NMR spectrum of NiL^n in presence of KPF_6 in CD_3CN .

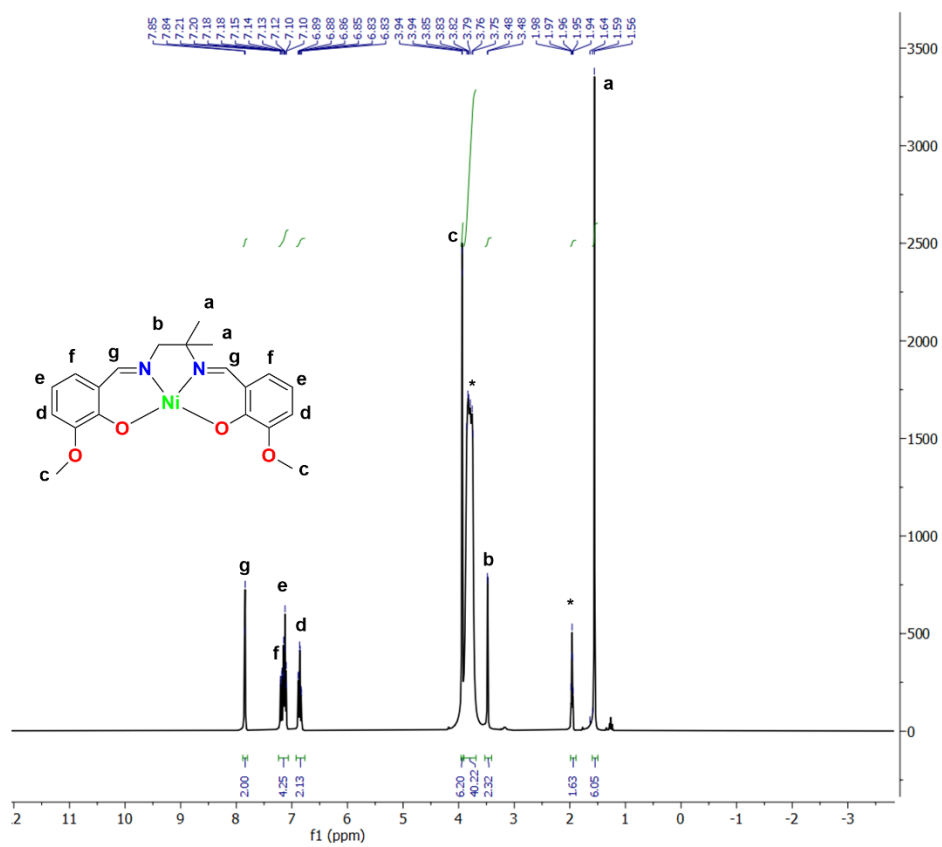


Fig. S33 1H -NMR spectrum of NiL^n in presence of $Mg(ClO_4)_2$ in CD_3CN .

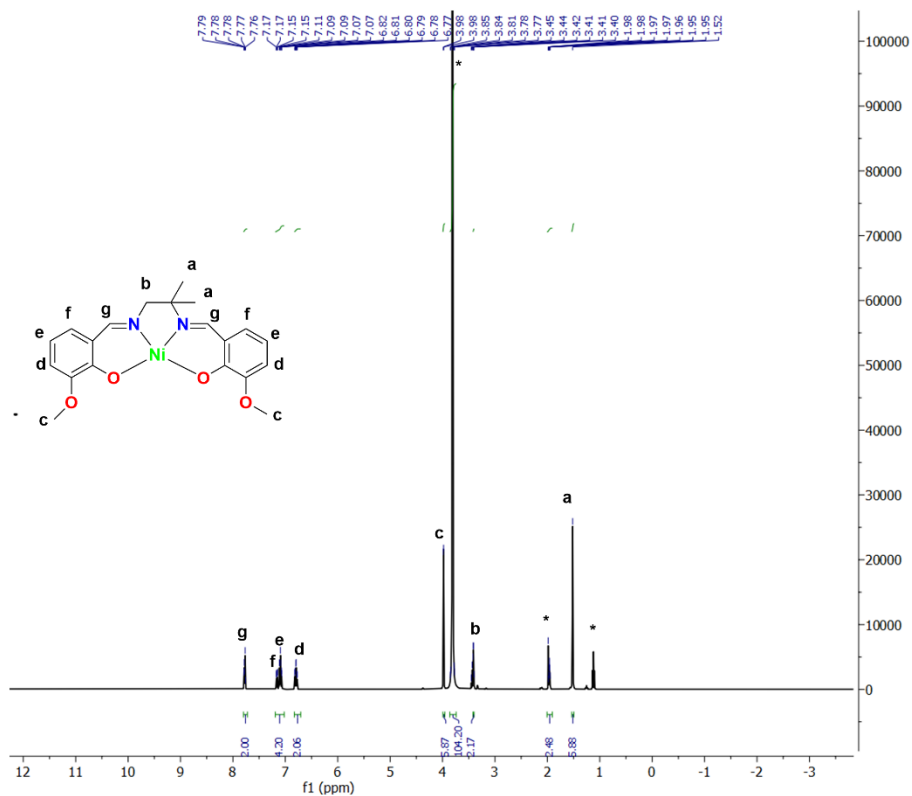


Fig. S34 ¹H-NMR spectrum of NiLⁿ in presence of Ca(ClO₄)₂ in CD₃CN.

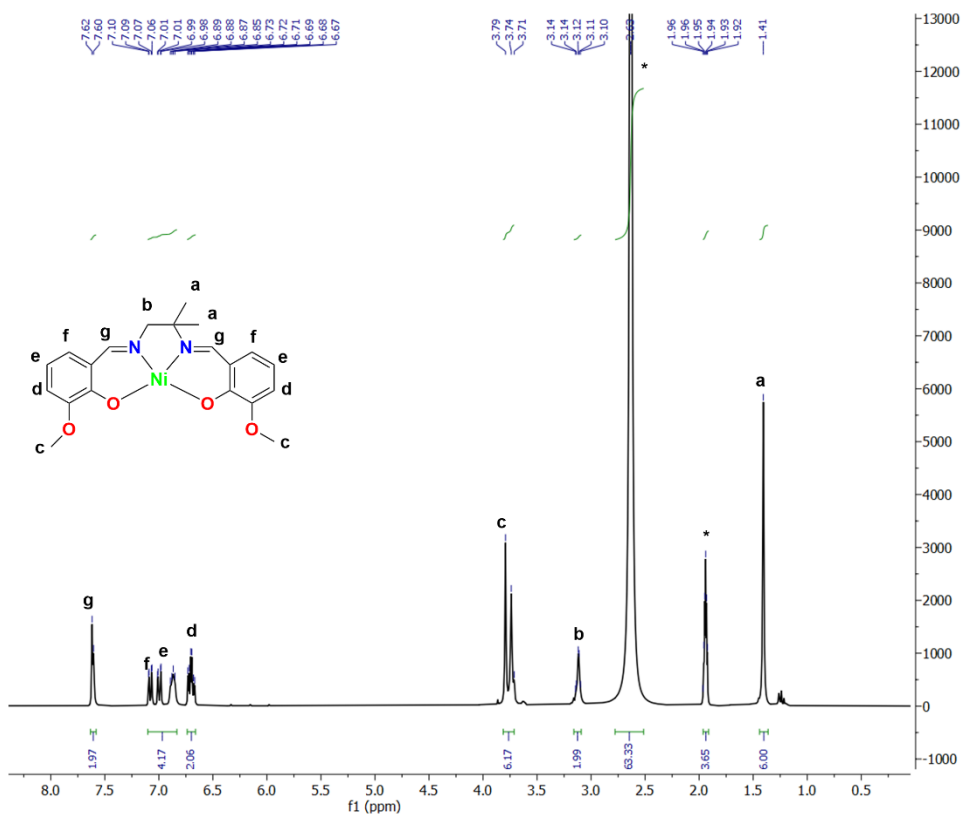


Fig. S35 ¹H-NMR spectrum of NiLⁿ in presence of Ba(ClO₄)₂ in CD₃CN.

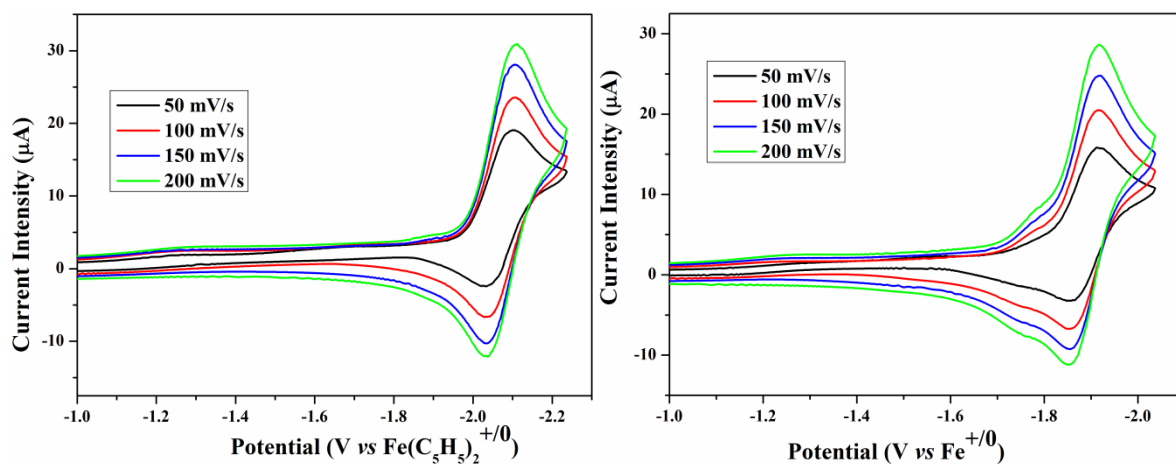
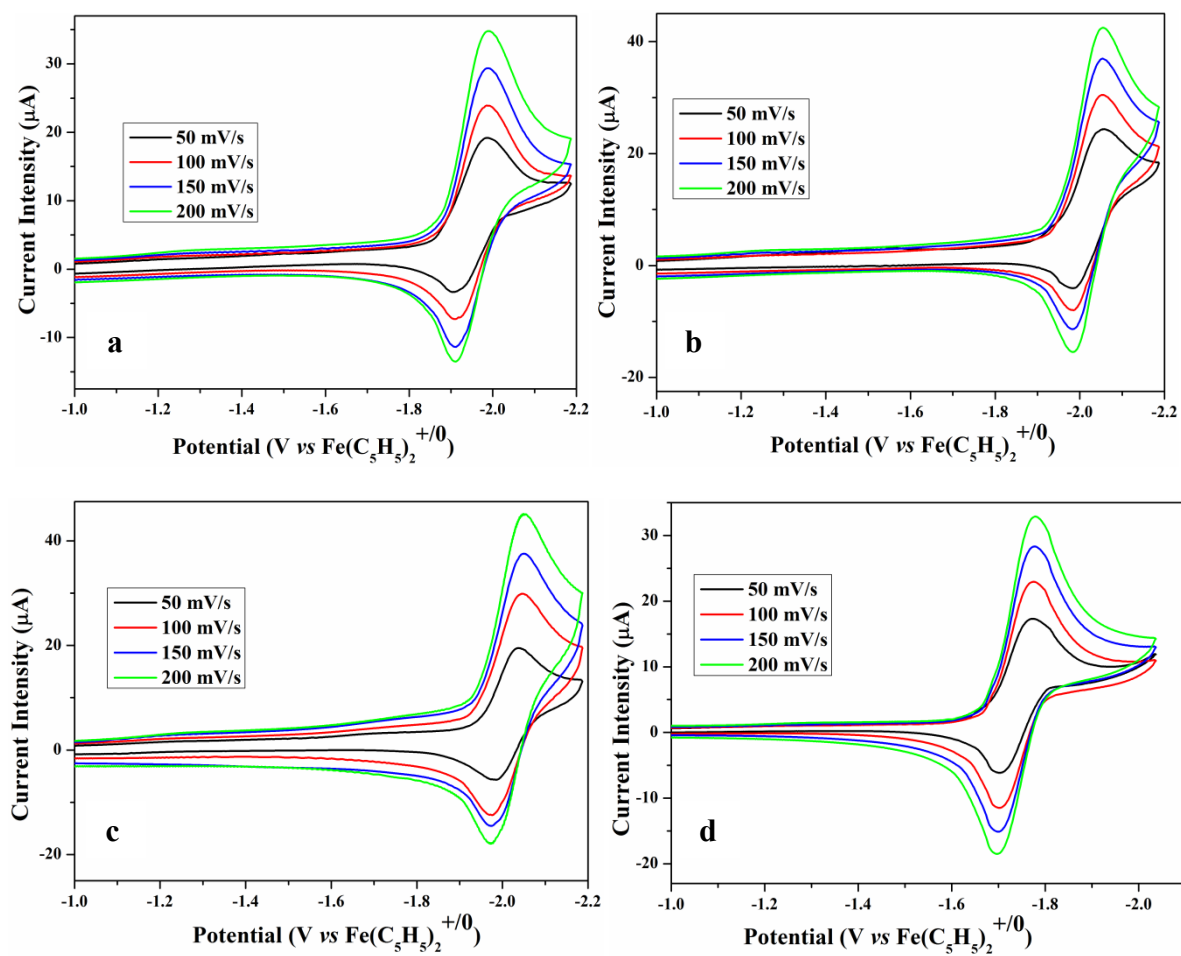


Fig. S36 Scan rate dependent cyclic voltammograms of NiL^{en} (left) and NiL^{n} (right) in acetonitrile.



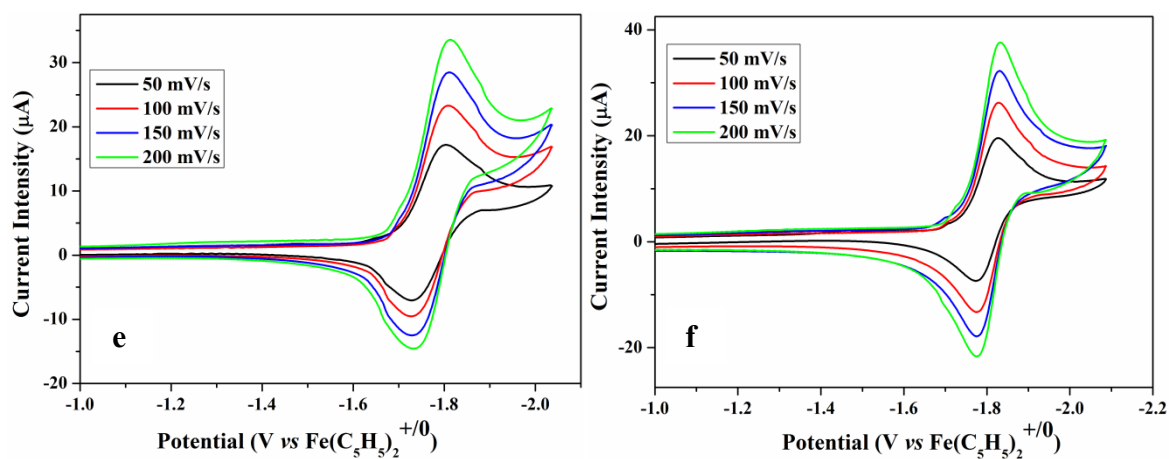
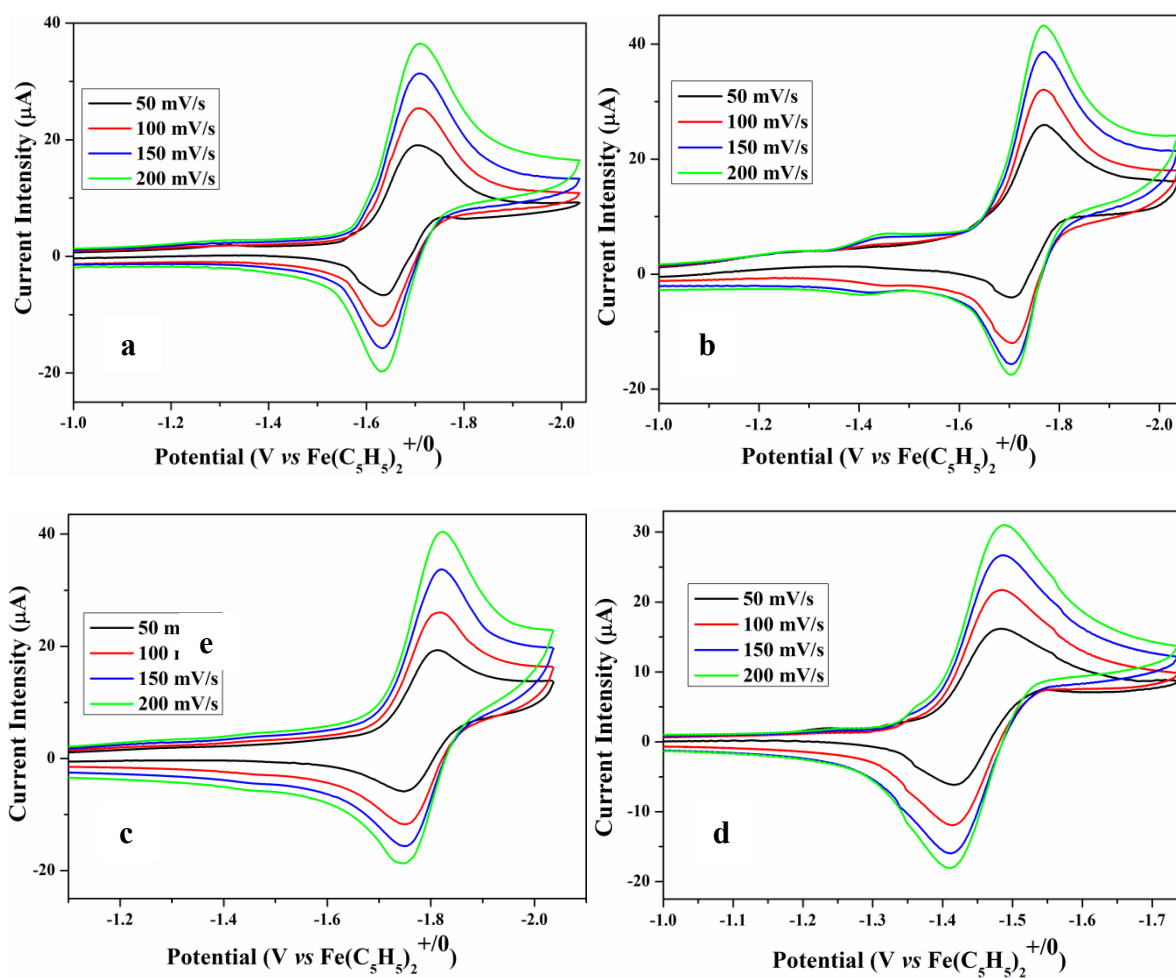


Fig. S37 Scan rate dependent cyclic voltammograms of NiL^{en} in presence of equivalent amount of Li^+ (a), Na^+ (b), K^+ (c), Mg^{2+} (d), Ca^{2+} (e) and Ba^{2+} (f) in acetonitrile.



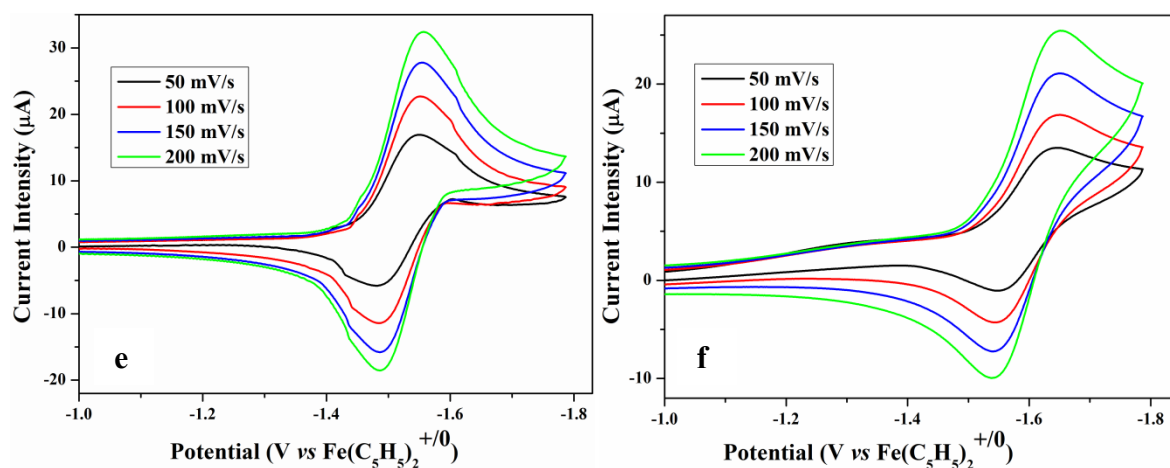


Fig. S38 Scan rate dependent cyclic voltammograms of NiL^{pn} in presence of equivalent amount of Li^+ (a), Na^+ (b), K^+ (c), Mg^{2+} (d), Ca^{2+} (e) and Ba^{2+} (f) in acetonitrile.

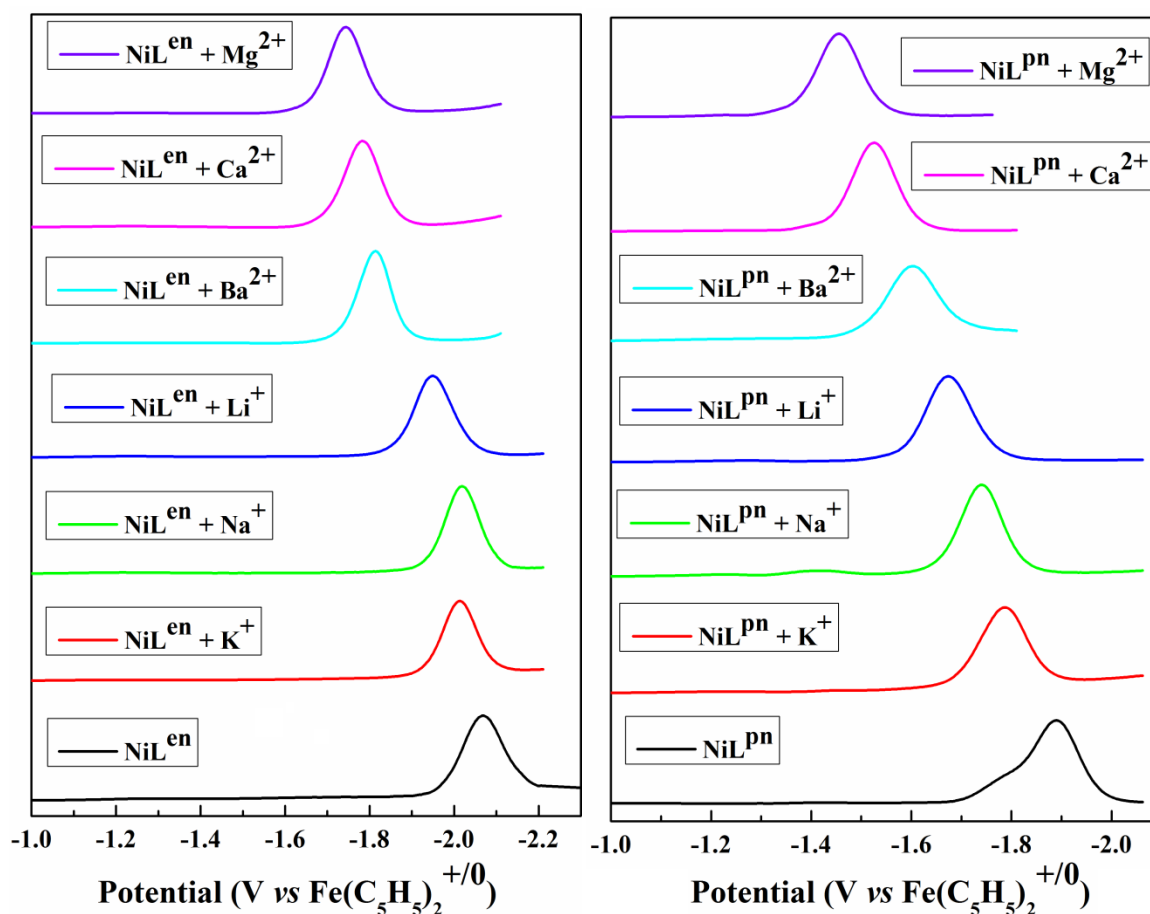


Fig. S39 Differential pulse voltammogram of $[\text{NiL}^{\text{en}}]$ (left) and $[\text{NiL}^{\text{pn}}]$ (right) in presence of equivalents amount of each of metal ions, Li^+ , Na^+ , K^+ , Mg^{2+} , Ca^{2+} and Ba^{2+} at 20 mV/s scan rate in acetonitrile.

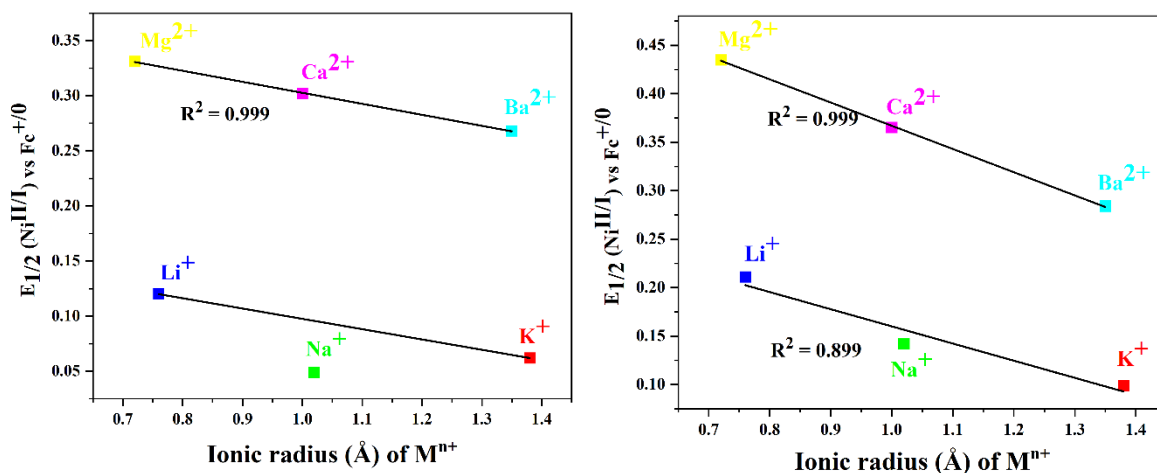


Fig. S40. Dependence of $E_{1/2}$ of Ni(II/I) couple on the ionic radius of the corresponding metal ions (left panel, $[\text{NiL}^{\text{en}}]$) and (right panel, $[\text{NiL}^{\text{pn}}]$).

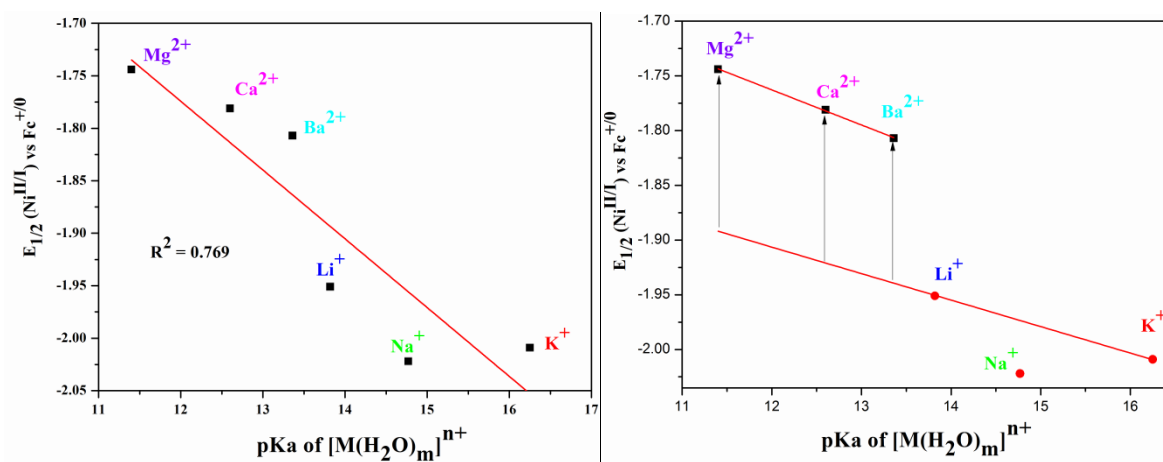


Fig. S41. Dependence of $E_{1/2}$ of Ni(II/I) couple on the Lewis acidity (pKa) of the corresponding $\text{M}(\text{aqua})^{n+}$ ions (left) and excess amount of shift by the bi-positive metal ions (right) for NiL^{en} .

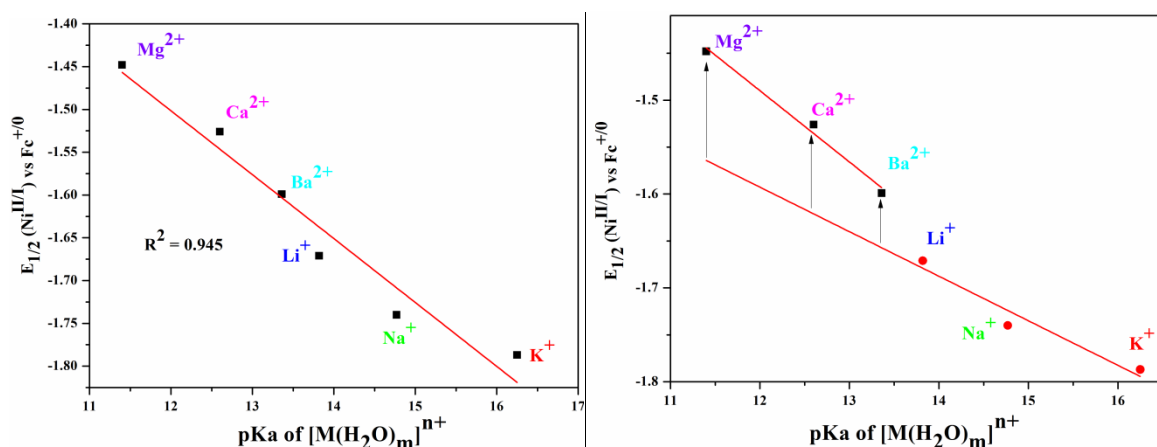


Fig. S42. Dependence of $E_{1/2}$ of Ni(II/I) couple on the Lewis acidity (pKa) of the corresponding $\text{M}(\text{aqua})^{n+}$ ions (left) and excess amount of shift by the bi-positive metal ions (right) for NiL^{pn} .

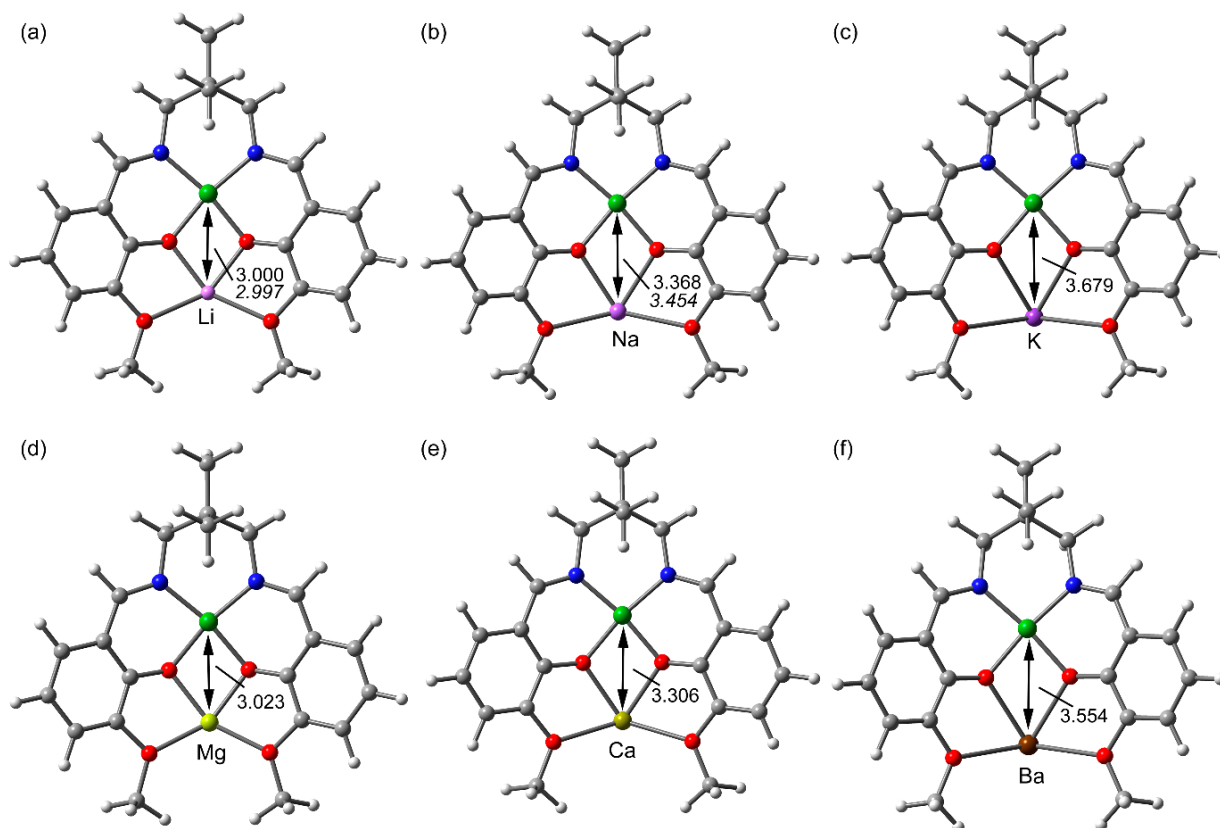


Fig. S43. (a-f) RI-BP86-D3/def2-TZVP optimized geometries of the NiL^{np} series of complexes used herein. Distances in Å. Values in *italics* corresponds to the experimental distances.

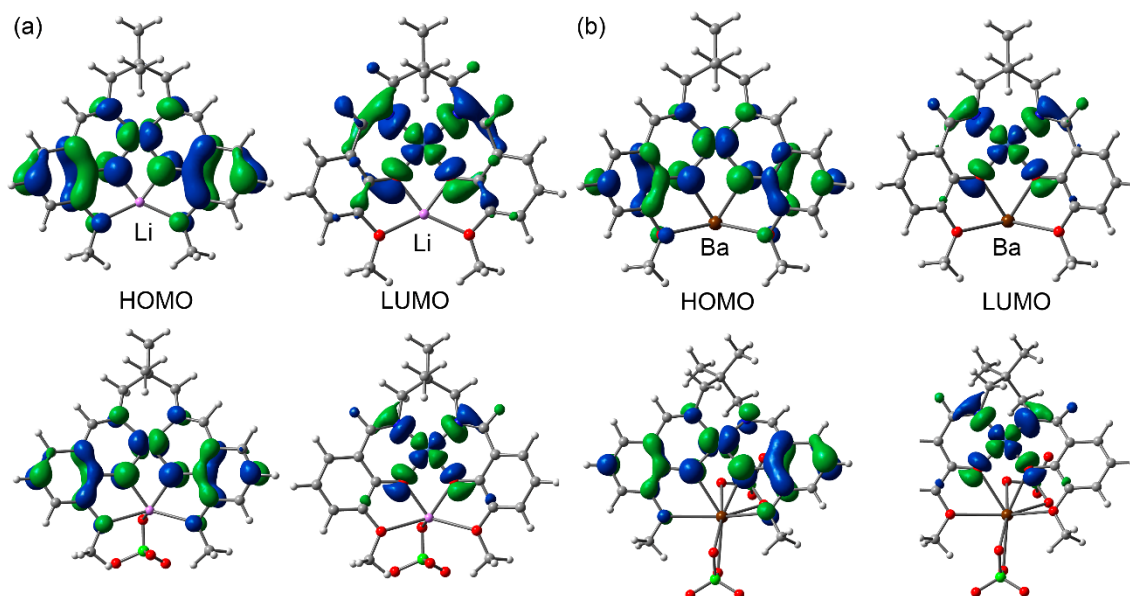


Fig. S44. Frontier orbital of Li (a) and Ba (b) NiL^{pn} complexes with (bottom) and without (top) the presence of the counterions (perchlorate anions)

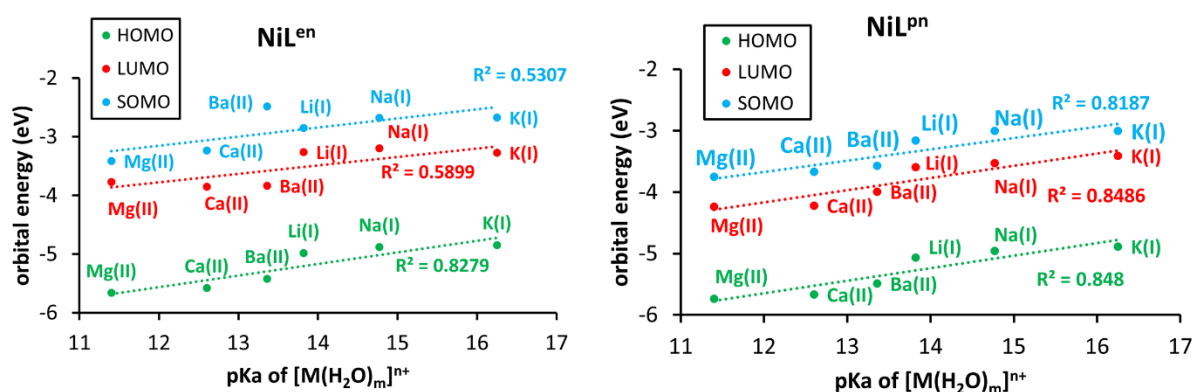


Fig. S45. Dependence of orbital energies of Ni(II/I) couple on the Lewis acidity (pKa) of the corresponding M(aqua)ⁿ⁺ ions for NiL^{en} (left) and NiL^{pn} (right) complexes.

Table S1. Bond parameters of complexes **1** and **2**.

Bond lengths (Å)					
	1	2		1	2
Ni1 – O11	1.840(5)	1.863(2)	Li1 – OC	1.954(15)	2.199(8)
Ni1 – OA	1.826(6)	1.841(2)	Li1 – O11	2.009(16)	2.054(6)
Ni1 – N19	1.826(7)	1.902(3)	Li1 – OA	2.072(14)	1.966(6)
Ni1 – NB	1.885(6)	1.893(3)	Li1 – O41	2.540(10)	2.104(6)
Li1 – O1	1.978(14)	1.907(6)			
Bond angles (°)					
O11 – Ni1 – OA	83.1(2)	82.04(9)	O11 – Li1 – OC	125.5(7)	139.5(3)
O11 – Ni1 – N19	96.9(2)	90.54(10)	OA – Li1 – O41	140.7(7)	133.5(3)
O11 – Ni1 – NB	176.5(3)	173.94(11)	OA – Li1 – OC	121.2(7)	75.7(3)
OA – Ni1 – N19	178.6(2)	170.79(10)	O41 – Li1 – OC	82.8(5)	105.6(3)
OA – Ni1 – NB	93.8(3)	91.98(11)	O1 – Li1 – O11	113.5(7)	119.8(4)
N19 – Ni1 – NB	86.3(3)	95.31(11)	O1 – Li1 – OA	106.9(6)	123.6(3)
O11 – Li1 – OA	73.2(5)	74.40(19)	O1 – Li1 – O41	89.7(5)	102.4(3)
O11 – Li1 – O41	67.6(4)	77.1(2)	O1 – Li1 – OC	110.8(8)	99.4(3)
A = 30 for 1 and 31 for 2 , B = 22 for 1 and 23 for 2 , C = 2 for 1 and 51 for 2					

Table S2. SHAPE analysis for the sodium centre in complex **3** (the lowest values are indicated in bold).

Geometry	Symmetry	3
Octagon	D8h	30.908
heptagonal pyramid	C7v	25.221
Hexagonal bipyramid	D6h	10.560
Cube	Oh	7.205
Square antiprism	D4d	6.066
Triangular dodecahedron	D2d	5.029
Johnson gyrobifastigium J26	D2d	10.491
Johnson elongated triangular bipyramid J14	D3h	24.341
Biaugmented trigonal prism J50	C2v	5.607
Biaugmented trigonal prism	C2v	4.688
Snub diphenoid J84	D2d	6.923
Triakis tetrahedron	Td	7.954
Elongated trigonal bipyramid	D3h	18.304

Table S3. SHAPE analysis for the barium centre in complex **4** (the lowest values are indicated in bold).

Geometry	Symmetry	4
Decagon	D10h	29.020
Enneagonal pyramid	C9v	25.215
Octagonal bipyramid	D8h	14.570
Pentagonal prism	D5h	7.687
Pentagonal antiprism	D5d	2.497
Bicapped cube J15	D4h	9.176
Bicapped square antiprism J17	D4d	12.123
Metabidiminished icosahedron J62	C2v	6.112
Augmented tridiminished icosahedron J64	C3v	16.085
Sphenocorona J87	C2v	12.192
Staggered Dodecahedron (2:6:2)	D2	5.348
Tetradecahedron (2:6:2)	C2v	7.687
Hexadecahedron (2:6:2) or (1:4:4:1)	D4h	6.204

Table S4. Bond lengths of complexes **3** and **4**.

Bond lengths (Å)

	3	4		3	4
Ni1 – O11	1.847(4)	1.863(9)	M 1 – O31	2.431(5)	2.722(8)
Ni1 – O31	1.840(4)	1.842(10)	M 1 – O41	2.583(4)	2.956(10)
Ni1 – N19	1.859(5)	1.877(12)	M 1 – O51	2.503(4)	2.994(8)
Ni1 – N23	1.865(5)	1.863(11)	M 1 – O61	2.415(5)	2.816(9)
Ni2 – O61	1.846(3)	1.837(9)	M 1 – O81	2.412(4)	2.702(9)
Ni2 – O81	1.839(4)	1.842(10)	M 1 – O91	2.570(4)	2.930(8)
Ni2 – N69	1.855(5)	1.835(13)	M 1 – O101	2.529(4)	3.022(8)
Ni2 – N73	1.857(5)	1.867(13)	M1 – O1		2.846(12)
M1 – O11	2.412(5)	2.857(9)	M1 – O2		2.855(13)
M = Na for 3 and Ba for 4					

Table S5. Bond angles of complex **3**.

Bond angles (Å) of 3			
O11 – Ni1 – O31	83.38(18)	O31 – Na1 – O51	63.47(15)
O11 – Ni1 – N19	93.6(2)	O31 – Na1 – O61	141.92(15)
O11 – Ni1 – N23	169.34(18)	O31 – Na1 – O81	137.03(15)
O31 – Ni1 – N19	168.3(2)	O31 – Na1 – O91	85.03(15)
O31 – Ni1 – N23	93.4(2)	O31 – Na1 – O101	87.51(16)
N19 – Ni1 – N23	91.5(2)	O41 – Na1 – O51	170.16(14)
O61 – Ni1 – O81	83.68(17)	O41 – Na1 – O61	89.93(15)
O61 – Ni1 – N69	93.01(19)	O41 – Na1 – O81	85.67(14)
O61 – Ni1 – N73	170.95(18)	O41 – Na1 – O91	106.57(14)
O81 – Ni1 – N69	170.68(18)	O41 – Na1 – O101	77.72(14)
O81 – Ni1 – N73	93.79(19)	O51 – Na1 – O61	91.12(15)
N69 – Ni1 – N73	90.8(2)	O51 – Na1 – O81	86.26(15)
O11 – Na1 – O31	60.84(14)	O51 – Na1 – O91	82.56(13)
O11 – Na1 – O41	62.19(14)	O51 – Na1 – O101	93.62(14)
O11 – Na1 – O51	123.58(17)	O61 – Na1 – O81	61.23(13)
O11 – Na1 – O61	129.26(14)	O61 – Na1 – O91	62.76(14)
O11 – Na1 – O81	143.97(15)	O61 – Na1 – O101	123.96(16)

O11 – Na1 – O91	84.46(14)	O81 – Na1 – O91	122.44(17)
O11 – Na1 – O101	92.39(16)	O81 – Na1 – O101	63.44(15)
O31 – Na1 – O41	120.07(16)	O91 – Na1 – O101	172.52(19)

Table S6. Bond angles of complex **4**.

Bond angles (Å) of 4			
O11 – Ni1 – O31	83.1(4)	O11 – Ba1 – O31	52.2(2)
O11 – Ni1 – N19	95.4(4)	O11 – Ba1 – O41	53.3(3)
O11 – Ni1 – N23	168.5(4)	O11 – Ba1 – O51	95.2(2)
O31 – Ni1 – N19	168.6(4)	O11 – Ba1 – O61	79.0(3)
O31 – Ni1 – N23	92.8(4)	O11 – Ba1 – O81	78.7(3)
N19 – Ni1 – N23	90.7(5)	O11 – Ba1 – O91	109.3(3)
O61 – Ni1 – O81	82.2(4)	O11 – Ba1 – O101	119.6(3)
O61 – Ni1 – N69	95.2(5)	O31 – Ba1 – O41	102.4(3)
O61 – Ni1 – N73	167.4(5)	O31 – Ba1 – O51	53.9(3)
O81 – Ni1 – N69	169.5(5)	O31 – Ba1 – O61	77.1(2)
O81 – Ni1 – N73	93.0(5)	O31 – Ba1 – O81	115.4(3)
N69 – Ni1 – N73	91.6(6)	O31 – Ba1 – O91	66.5(2)
O1 – Ba1 – O2	65.9(3)	O31 – Ba1 – O101	169.0(3)
O1 – Ba1 – O11	165.7(3)	O41 – Ba1 – O51	117.9(3)
O1 – Ba1 – O31	119.0(3)	O41 – Ba1 – O61	107.3(3)
O1 – Ba1 – O41	127.9(3)	O41 – Ba1 – O81	66.1(3)
O1 – Ba1 – O51	71.6(3)	O41 – Ba1 – O91	159.4(3)
O1 – Ba1 – O61	111.4(3)	O41 – Ba1 – O101	73.0(3)
O1 – Ba1 – O81	115.3(3)	O51 – Ba1 – O61	117.7(2)
O1 – Ba1 – O91	71.9(3)	O51 – Ba1 – O81	168.6(3)
O1 – Ba1 – O101	70.6(3)	O51 – Ba1 – O91	70.7(3)
O2 – Ba1 – O11	106.0(3)	O51 – Ba1 – O101	137.1(3)
O2 – Ba1 – O31	114.8(3)	O61 – Ba1 – O81	52.0(3)
O2 – Ba1 – O41	68.9(3)	O61 – Ba1 – O91	54.4(3)
O2 – Ba1 – O51	73.3(3)	O61 – Ba1 – O101	94.5(3)

O2 – Ba1 – O61	167.9(3)	O81 – Ba1 – O91	102.0(3)
O2 – Ba1 – O81	117.5(3)	O81 – Ba1 – O101	53.6(3)
O2 – Ba1 – O91	131.0(3)	O91 – Ba1 – O101	114.6(2)
O2 – Ba1 – O101	73.4(3)		

Table S7. Comparison of bond lengths of heterometallic nickel complexes of N₂O₄ donor Schiff base ligands derived from propylenediamine and its derivative.

Complex Code	Average bond length of Ni(II) with N ₂ O ₂ donor atoms of ligand [τ 4]	Average bond length of guest metal with O ₄ donor atoms of ligand	Ni(II) –guest metal ion distance	Reference
XEDBEN	1.886(3) [0.126]	2.371(4) [Ni-Na]	3.467(2)	1
XEDBUD	1.859(5) [0.225]	2.468(4) [Ni ₂ Na]	3.501(2)	1
XEDCOY	1.868(4) [0.160]	2.799(4) [Ni ₃ K ₂]	3.709(1)	1
XEDCEO	1.872(3) [0.175]	3.141(1) [Ni ₂ Cs]	4.004(1)	1
XEDBEN03	1.951(2) [0.124]	2.386(3) [Ni-Na]	3.467(2)	2
YUKTEG	1.884(5) [0.089]	2.486(5) [Ni ₂ Na]	3.571(2)	3
YUKTIK	1.884(5) [0.162]	2.498(6) [Ni ₂ Na]	3.649(2)	3
YUKTOQ	1.853(4) [0.172]	2.504(4) [Ni ₂ Na]	3.446(2)	3
YUKTUW	1.863(5) [0.153]	2.499(5) [Ni ₂ Na]	3.468(3)	3
EBIBUO	1.859(1) [0.093]	2.459(2) [Ni ₂ Na]	3.373(7)	4
EBIBOI	1.841(4) [0.171]	2.931(4) [Ni ₂ K]	3.677(1)	4
EBIBIC	1.861(2) [0.174]	2.562(2) [Ni ₃ K ₂]	3.693(1)	4
FOFLIX	1.885(2) [0.117]	2.353(2) [Ni-Na]	3.429(1)	5
Complex 2	1.875(2) [0.108]	2.081(6) [Ni-Li]	2.997(5)	This work
Complex 3	1.853(4) [0.145]	2.482(4) [Ni ₂ Na]	3.455(3)	This work
Complex 4	1.862(1) [0.163]	2.875(8) [Ni ₂ Ba]	3.751(2)	This work

Table S8. Comparison of bond lengths of heterometallic nickel complexes of N₂O₄ donor Schiff base ligands derived from ethylenediamine and its derivative.

Complex Code	Average bond length of Ni(II) with N ₂ O ₄ donor atoms of ligand[t4]	Average bond length of guest metal with O ₄ donor atoms of ligand	Ni(II) –guest metal ion distance	Reference
VEFHOH	1.843(3) [0.041]	2.164(7) [Ni-Li]	3.012(7)	6
VEFMUS	1.845(1) [0.051]	3.692(1) [Ni ₂ K]	3.731(1)	6
QEWDEE	1.842(2) [0.030]	2.113(7) [Ni ₂ Li ₂]	2.976(6)	7
VEKRIP	1.846(2) [0.036]	3.118(2) [Ni ₂ Cs]	4.014(1)	7
VILYEW01	1.843(3) [0.022]	2.456(3) [Ni-Na]	3.390(2)	7
ECAYOY	1.842(1) [0.028]	2.428(1) [Ni-Na]	3.324(1)	8
ECAYUE	1.835(2) [0.047]	2.485(2) [Ni ₂ Li]	3.445(1)	8
ECAYEO	1.831(4) [0.034]	2.284(9) [Ni-Li]	2.991(9)	8
ECAZAL	1.835(2) [0.039]	2.931(2) [Ni ₂ Rb]	3.729(1)	8
ECAZEP	1.847(4) [0.043]	3.083(3) [Ni ₂ Cs]	3.901(1)	8
ECAZIT	1.832(1) [0.032]	3.362(1) [Ni-Mg]	3.206(1)	8
ECAZoz	1.832(3) [0.027]	2.439(3) [Ni-Ca]	3.403(1)	8
JAWBAO	1.839(5) [0.029]	2.369(1) [Ni-Na]	3.355(6)	9
ROMXOJ	1.846(2) [0.052]	2.89(1) [Ni ₂ Ba]	3.774(3)	10
ROMXUP	1.844(2) [0.030]	2.462(2) [Ni-Ca]	3.393(1)	10
ROMYAW	1.828(4) [0.058]	2.261(4) [Ni-Mg]	3.088(2)	10
ROMYEA	1.851(3) [0.017]	2.591(3) [Ni-Sr]	3.591(1)	10
VILXUL	1.841(3) [0.021]	2.424(4) [Ni-Na]	3.345(2)	11
VILYAS	1.832(6) [0.023]	2.485(2) [Ni ₂ Na]	3.422(2)	11
VILYEW	1.835(2) [0.021]	2.456(2) [Ni-Na]	3.387(1)	11
XEMJOQ	1.841(4) [0.019]	2.962(4) [Ni ₄ K ₃]	3.753(2)	12
XAJCET	1.842(2) [0.039]	2.445(3) [Ni-Na]	3.390(1)	13
XAJCAP	1.841(3) [0.039]	2.458(3) [Ni ₂ Na ₂]	3.367(1)	13
Complex 1	1.844(6) [0.036]	2.207(1) [Ni-Li]	3.008(2)	This work

Table S9. UV-*vis* data of NiL^{en} in presence of redox innocent metal ions.

Ethylenediamine (five-membered ring) chelate							
Adducts	CT band position (nm)			λ_{iso} (nm)	d-d band position (nm)	NiL ^{en} : M ⁿ⁺	Stability constant (K _b) for 1:1 complex
	ILCT	MLCT					
NiL ^{en}	253	346	411		552		
NiL ^{en} + Li ⁺	246.5	341	400	249, 349, 407.5	537	1:1	7.87 x 10 ³
NiL ^{en} + Na ⁺	248	342	402	250, 349.5, 405	542	2:1	
NiL ^{en} + K ⁺	250	343	404	251.5, 348.5, 407	549	1:1	5.59 x 10 ³
NiL ^{en} + Mg ²⁺	237	332.5	381	241, 342, 391	526	2:1	
NiL ^{en} + Ca ²⁺	241	334	384	244.5, 343, 395	535	2:1	

NiL ^{en} + Ba ²⁺	245	338	392	247, 342.5, 397	547	2:1	
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Table S10. UV-vis data of NiL^{pn} in presence of redox innocent metal ions.

Propylenediamine (six-membered ring) chelate							
Adducts	CT band position (nm)			λ_{iso} (nm)	d-d band position (nm)	NiL ^{en} : M ⁿ⁺	Stability constant (K _b) for 1:1 complex
	ILCT	MLCT					
NiL ^{pn}	257	353.5	418		591		
NiL ^{pn} + Li ⁺	250	346	406	252, 355.5, 409.5	580	1:1	6.89 x 10 ³
NiL ^{pn} + Na ⁺	251	347.5	408	254, 356.5, 414	582	2:1	
NiL ^{pn} + K ⁺	253	348.5	411.5	255, 357, 415	585	2:1	
NiL ^{pn} + Mg ²⁺	231	349		239.5, 382.5	564	1:1	1.41 x 10 ⁴
NiL ^{pn} + Ca ²⁺	233	352		242, 378,	556	2:1	
NiL ^{pn} + Ba ²⁺	235	350		243.5, 395	579	2:1	

Table S11. Comparison of bond lengths of mononuclear nickel complexes of N₂O₄ donor Schiff base ligands.

Code of Ni(II) complex of Salen type N ₂ O ₄ ligand	Average bond length of Ni(II) with N ₂ O ₂ donor atoms of ligand[τ_4]	Reference	Code of Ni(II) complex of Salpn type N ₂ O ₄ ligand	Average bond length of Ni(II) with N ₂ O ₂ donor atoms of ligand[τ_4]	Reference
ARARIV	1.857(7) [0.064]	14	CEHZAT	1.863(3) [0.143]	29
AXUTOE	1.856(5) [0.096]	15	HAIYOK	1.884(4) [0.115]	30
AXUTUK	1.862(2) [0.047]	15	IQEGER	1.859(3) [0.137]	31
BOCVEX	1.853(3) [0.019]	16	LOSBEB	1.866(1) [0.272]	32
GECFEB	1.865(1) [0.101]	17	PONZOK	1.868(3) [0.264]	33
GECFIF	1.863(6) [0.109]	17			
GECFOL	1.853(1) [0.102]	17			
IDELUZ	1.854(3) [0.072]	18			
IDUPEG	1.865(2) [0.021]	19			
KOHHAQ	1.845(2) [0.049]	20			

KOHHIY	1.851(5) [0.036]	20			
MABNEK	1.848(2) [0.079]	21			
QIYVAX	1.837(2) [0.063]	22			
SULZUU	1.841(6) [0.042]	23			
TEJGIZ	1.843(2) [0.017]	24			
TUMMUL	1.844(2) [0.039]	25			
TUZDOK	1.858(2) [0.032]	26			
ECA YEO	1.838(5) [0.024]	8			
ECAZIT	1.844(4) [0.054]	8			
VOHSIV	1.855(1) [0.027]	27			
VOHSIV01	1.857(1) [0.027]	28			
TUZDUQ	1.855(1) [0.039]	26			
TUZFAY	1.853(2) [0.028]	26			

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Cartesian Coordinates

Ni(I)L^{en}

Ni	-1.8234017	6.4005139	7.0530212
O	0.0930587	6.8533905	7.2111350

O	-1.3393465	4.7479576	6.1441534
O	-0.1278597	2.6111482	5.2102841
O	2.7008230	6.8412324	7.5265617
N	-3.6837721	5.9228221	7.1387210
N	-2.3470189	8.0823087	7.7326589
C	-2.0612879	3.6840385	6.0538300
C	0.5830564	7.8415401	7.8701881
C	-1.4556487	2.4685222	5.5496702
C	-4.4765529	6.9066639	7.9219428
C	-4.1375681	4.6863148	7.0506642
H	-5.1071362	4.4358215	7.5126302
C	2.0200439	7.9015794	8.0785703
C	-3.4515126	3.5857901	6.4488591
C	-1.6065566	8.9827707	8.3280809
H	-2.1088882	9.8463126	8.8016094
C	-0.1799141	8.9342473	8.4398683
C	-4.3881356	6.5730350	9.4218627
H	-3.3318137	6.5556269	9.7244526
H	-4.8201108	5.5820206	9.6220631
H	-4.9261350	7.3203471	10.0272734
C	0.4755774	9.9824300	9.1404619
H	-0.1376444	10.7892456	9.5543123
C	-3.5318695	1.2242531	5.8022958
H	-4.0834499	0.2886143	5.6936369
C	-4.1433175	2.3497174	6.3159992
H	-5.1909661	2.3083203	6.6304150
C	-3.7864608	8.2630592	7.6594615
H	-4.1532849	9.0269612	8.3727518
H	-4.0460470	8.5911425	6.6372508
C	2.6232926	8.9462537	8.7633597
H	3.7056786	8.9673649	8.8942183
C	-2.1732117	1.2874032	5.4086817
H	-1.6970524	0.3959501	4.9993010
C	1.8455977	10.0004605	9.3028188
H	2.3359727	10.8152559	9.8378282
C	4.1050556	6.8207385	7.6813668
H	4.5889399	7.6972120	7.2086483
H	4.4513099	5.9064139	7.1824979
H	4.4063735	6.7887178	8.7460643
C	-5.9384248	6.9864570	7.4603547
H	-6.4419628	7.8435686	7.9343359
H	-6.4999186	6.0809101	7.7288639
H	-5.9846364	7.1091396	6.3686857
C	0.5445149	1.4657641	4.7303574
H	0.5436325	0.6413250	5.4695886
H	1.5797116	1.7792264	4.5429116
H	0.1046712	1.0872024	3.7873874

Ni (I) L^{en} + Li⁺

Ni	-1.9374781	6.5470018	6.9488428
O	-0.0814782	7.1470128	6.7067899
O	-1.2185715	4.8449596	6.3349375
O	0.0868185	2.7966693	5.4469189
O	2.3703157	6.6268965	7.3062738
N	-3.6694065	5.9471507	7.2797804
N	-2.4631048	8.2640404	7.5265740
C	-1.9326409	3.7562047	6.1785486
C	0.4622201	7.9710951	7.5759010
C	-1.2624244	2.5943130	5.6814271
C	-4.4980643	6.9544683	8.0077609
C	-4.1046192	4.7387286	7.0468702
H	-5.1418686	4.4796229	7.3046103
C	1.8325369	7.7713719	7.9021367
C	-3.3275956	3.6549360	6.4843373
C	-1.6941048	9.0984555	8.1911850
H	-2.1668276	9.8677538	8.8235127
C	-0.2565542	9.0130120	8.2463400
C	-4.2836002	6.7161415	9.5123839
H	-3.2137942	6.7899201	9.7512781
H	-4.6328736	5.7128907	9.7934477
H	-4.8358753	7.4602861	10.1046414
C	0.4702310	9.8904333	9.0929883
H	-0.0689292	10.6998477	9.5907631
C	-3.3147709	1.3153418	5.7662893
H	-3.8404302	0.3748091	5.6020949
C	-3.9853961	2.4163165	6.2635288
H	-5.0496653	2.3438847	6.4994885

C	-3.9140426	8.3424562	7.6161042
H	-4.2542321	9.1010182	8.3447482
H	-4.3039395	8.6195186	6.6223351
C	2.5226268	8.6455362	8.7308380
H	3.5826034	8.5105167	8.9420269
C	-1.9375140	1.4002729	5.4735609
H	-1.4177296	0.5233775	5.0896409
C	1.8264966	9.7276614	9.3148119
H	2.3654054	10.4207356	9.9606415
C	3.7418186	6.3429305	7.5852415
H	4.3980223	7.1506956	7.2216769
H	3.9797426	5.4159089	7.0497180
H	3.9100498	6.1955389	8.6651841
C	-5.9874325	6.9083483	7.6490808
H	-6.5012883	7.7748112	8.0893339
H	-6.4779299	6.0072167	8.0413452
H	-6.1284973	6.9384360	6.5593522
C	0.8232018	1.6974000	4.9150048
H	0.8186736	0.8346866	5.6029086
H	1.8524834	2.0532656	4.7882671
H	0.4249411	1.3818921	3.9359878
Li	0.5428917	5.4513123	6.3448407

Ni (I) L^{en} + Na⁺

Ni	-1.8646853	6.3601650	7.2082827
O	0.0452856	6.8741470	7.1355073
O	-1.2407624	4.6008939	6.6058940
O	-0.0250566	2.5736005	5.5125644
O	2.6229068	6.7484140	7.5469952
N	-3.6576031	5.8249576	7.4145784
N	-2.3910366	8.1104983	7.6622516
C	-2.0165820	3.6116485	6.2550779
C	0.5596467	7.8869044	7.7844783
C	-1.4075816	2.4636814	5.6500650
C	-4.4836175	6.8704652	8.0818328
C	-4.1745152	4.6949840	7.0124299
H	-5.2592007	4.5345632	7.0946202
C	1.9707730	7.8908685	8.0208112
C	-3.4391850	3.5925640	6.4351172
C	-1.6426812	9.0246698	8.2314902
H	-2.1359452	9.8668690	8.7455946
C	-0.2034267	8.9914039	8.2957732
C	-4.3330260	6.6591676	9.5988658
H	-3.2718970	6.7135265	9.8774890
H	-4.7145902	5.6686629	9.8827763
H	-4.8920178	7.4258293	10.1551845
C	0.4754942	10.0517494	8.9489312
H	-0.1137931	10.8907079	9.3271444
C	-3.5494288	1.3564478	5.4469511
H	-4.1298090	0.4874648	5.1378480
C	-4.1702849	2.4499184	6.0206666
H	-5.2534009	2.4471510	6.1643305
C	-3.8426519	8.2285962	7.6823901
H	-4.1924436	9.0182485	8.3740425
H	-4.1796130	8.4880925	6.6648702
C	2.6090747	8.9503568	8.6508388
H	3.6889460	8.9542219	8.7924092
C	-2.1510296	1.3607317	5.2580130
H	-1.6725721	0.4928191	4.8059977
C	1.8482311	10.0442804	9.1151388
H	2.3511967	10.8760590	9.6081798
C	4.0298404	6.6776329	7.7689835
H	4.5629623	7.4915742	7.2495248
H	4.3599442	5.7148211	7.3583592
H	4.2724704	6.7143906	8.8443786
C	-5.9625571	6.8735718	7.6797160
H	-6.4532719	7.7677520	8.0899214
H	-6.4982905	5.9998530	8.0753665
H	-6.0757439	6.8893659	6.5861003
C	0.6472117	1.4753528	4.9007748
H	0.5265282	0.5487504	5.4873404
H	1.7106681	1.7433663	4.8679681
H	0.2865676	1.3021732	3.8726290
Na	0.9389527	4.9531661	6.5258052

Ni (I) L^{en} + K⁺

Ni	-1.8001869	6.2969748	7.2390442
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O	0.1422071	6.8220629	7.3058586
O	-1.2414770	4.5109100	6.5597906
O	-0.1169975	2.4107934	5.4219103
O	2.7576635	6.8802918	7.6779795
N	-3.6272436	5.7894725	7.4128359
N	-2.3399333	8.0604304	7.6832117
C	-2.0508323	3.5476666	6.2135389
C	0.6150481	7.8908649	7.8891516
C	-1.5009480	2.3728639	5.5912083
C	-4.4428468	6.8443366	8.0756906
C	-4.1729680	4.6759562	7.0091529
H	-5.2598650	4.5369386	7.1051244
C	2.0309009	7.9898641	8.1150651
C	-3.4742141	3.5628962	6.4136264
C	-1.6211920	9.0038469	8.2323322
H	-2.1383250	9.8693677	8.6818732
C	-0.1855608	8.9990997	8.3380352
C	-4.2907228	6.6484665	9.5944557
H	-3.2280304	6.6885560	9.8690717
H	-4.6875044	5.6673837	9.8903667
H	-4.8355588	7.4302298	10.1440946
C	0.4377664	10.1170603	8.9480555
H	-0.1947176	10.9441040	9.2801452
C	-3.6853371	1.3377409	5.4175241
H	-4.3001263	0.4909928	5.1132694
C	-4.2534904	2.4496391	6.0075448
H	-5.3331898	2.4871004	6.1722659
C	-3.7901534	8.1865388	7.6554775
H	-4.1541923	8.9993258	8.3122565
H	-4.0967708	8.4147393	6.6210258
C	2.6130685	9.1054331	8.7010673
H	3.6918279	9.1663966	8.8387664
C	-2.2915635	1.2996490	5.2073763
H	-1.8505932	0.4184252	4.7433617
C	1.8065387	10.1818530	9.1239614
H	2.2693642	11.0537517	9.5858697
C	4.1654309	6.9115188	7.8948472
H	4.6444577	7.7413406	7.3477205
H	4.5597769	5.9594472	7.5157688
H	4.4094326	6.9991874	8.9671983
C	-5.9238327	6.8632635	7.6804347
H	-6.3995032	7.7673686	8.0867814
H	-6.4702414	6.0005987	8.0854601
H	-6.0435218	6.8726008	6.5873773
C	0.4839492	1.2750344	4.8055887
H	0.3242388	0.3578066	5.3978470
H	1.5607077	1.4832193	4.7540510
H	0.1003233	1.1156065	3.7832763
K	1.2973377	4.7380847	6.4145628

Ni (I) L^{en} + Mg²⁺

Ni	-1.9942064	6.3598275	7.3283207
O	-0.2051958	6.8572490	6.6841738
O	-1.2383221	4.5537295	7.4399795
O	0.2232054	3.1846778	5.8395106
O	2.1591810	6.2017303	7.4341158
N	-3.7299750	5.7770236	7.6784202
N	-2.5224514	8.1311490	7.5088904
C	-1.9154657	3.6477429	6.7265380
C	0.4030407	7.7809117	7.4380239
C	-1.1598709	2.8080278	5.8879478
C	-4.5673185	6.8907098	8.2105740
C	-4.1832208	4.6203758	7.2763487
H	-5.2635524	4.4271023	7.2527215
C	1.7319314	7.5170583	7.8166295
C	-3.3351974	3.5674275	6.7221866
C	-1.7112529	9.0761559	7.9109463
H	-2.1268901	9.9946872	8.3512849
C	-0.2608247	8.9375500	7.9375647
C	-4.3528410	6.8971414	9.7351075
H	-3.2862904	7.0221316	9.9682441
H	-4.6913956	5.9479030	10.1708671
H	-4.9186658	7.7172485	10.1978423
C	0.5344503	9.8762230	8.6366743
H	0.0655419	10.7894611	9.0072545
C	-3.1326009	1.6061978	5.2694271
H	-3.6045148	0.7876765	4.7280298

C	-3.9105262	2.4936469	6.0039746
H	-4.9963991	2.3831135	6.0026795
C	-3.9789018	8.2125115	7.6012534
H	-4.3181091	9.0746179	8.2006598
H	-4.3670398	8.3262416	6.5767328
C	2.4958275	8.4351424	8.5192797
H	3.5345810	8.2484056	8.7855838
C	-1.7368241	1.7722587	5.1707278
H	-1.1536166	1.1010942	4.5429397
C	1.8795892	9.6451205	8.8967735
H	2.4660554	10.3890225	9.4339593
C	3.5265683	5.8427893	7.7558445
H	4.2208326	6.5256275	7.2490981
H	3.6733455	4.8223087	7.3839443
H	3.6822091	5.8688900	8.8427336
C	-6.0532584	6.7886971	7.8639388
H	-6.5748449	7.6972641	8.1942931
H	-6.5281961	5.9404406	8.3752864
H	-6.2082361	6.6823542	6.7807275
C	1.0864856	2.3787166	4.9983842
H	1.0974549	1.3416889	5.3583266
H	2.0904037	2.8102973	5.0830821
H	0.7491759	2.4227033	3.9541999
Mg	0.5145256	5.0570287	6.7802530

Ni (I) L^{en} + Ca²⁺

Ni	-1.9180794	6.3517529	7.3058131
O	-0.0071321	6.8507372	7.0805499
O	-1.2479121	4.5508375	6.8982045
O	0.0456052	2.7236290	5.6625838
O	2.5060542	6.5992269	7.5206514
N	-3.7030549	5.7973966	7.5066497
N	-2.4266991	8.1095784	7.6973608
C	-2.0178437	3.5856525	6.4022377
C	0.5369643	7.8782886	7.7312864
C	-1.3552442	2.5333495	5.7330826
C	-4.5327709	6.8687893	8.1363321
C	-4.2065940	4.6808617	7.0610762
H	-5.2942743	4.5298949	7.0664352
C	1.9268971	7.8122104	7.9705070
C	-3.4361604	3.5831891	6.4946892
C	-1.6581862	9.0502554	8.1763380
H	-2.1203170	9.9400559	8.6311141
C	-0.2077615	8.9891086	8.2190982
C	-4.3913850	6.6904130	9.6589027
H	-3.3345340	6.7528711	9.9523192
H	-4.7770952	5.7088586	9.9648712
H	-4.9566131	7.4691314	10.1893999
C	0.5127949	10.0313900	8.8511043
H	-0.0382029	10.8976040	9.2216810
C	-3.4484763	1.4255322	5.3383865
H	-4.0023207	0.5788617	4.9351699
C	-4.1224865	2.4692719	5.9537292
H	-5.2116192	2.4429536	6.0204403
C	-3.8845520	8.2216382	7.7096699
H	-4.2384343	9.0264526	8.3769273
H	-4.2062065	8.4566253	6.6826563
C	2.6154656	8.8439380	8.5906478
H	3.6908733	8.8034794	8.7537436
C	-2.0461557	1.4504014	5.2108059
H	-1.5368243	0.6302068	4.7079229
C	1.8876068	9.9707477	9.0192765
H	2.4164953	10.7911904	9.5022860
C	3.9330918	6.4708548	7.6962270
H	4.4641056	7.2595896	7.1445227
H	4.2104538	5.4915869	7.2857056
H	4.2000781	6.5079968	8.7620335
C	-6.0052122	6.8611549	7.7198489
H	-6.5046396	7.7568794	8.1135859
H	-6.5386212	5.9917315	8.1269450
H	-6.1139102	6.8631560	6.6258630
C	0.7951424	1.6898409	4.9898115
H	0.6737753	0.7252367	5.5032472
H	1.8491413	1.9915347	5.0319020
H	0.4821696	1.6022928	3.9393276
Ca	0.8510042	4.9288632	6.6393294

Ni (I) L^{en} + Ba²⁺

Ni	-1.8254324	6.2762829	7.3569586
O	0.1484223	6.7591361	7.4397811
O	-1.2418970	4.4674037	6.6913332
O	-0.0921266	2.4146024	5.5755596
O	2.7432519	6.8518853	7.6469398
N	-3.6649993	5.7780221	7.4316548
N	-2.3424866	8.0298768	7.8467339
C	-2.0709629	3.5186559	6.2546566
C	0.6383324	7.8841779	7.9620001
C	-1.4961022	2.3761239	5.6392894
C	-4.4871546	6.8271458	8.1051773
C	-4.2059881	4.6906999	6.9704581
H	-5.2960636	4.5610648	7.0142162
C	2.0470856	7.9885124	8.0968995
C	-3.4889976	3.5808572	6.3699446
C	-1.6093270	8.9959232	8.3149327
H	-2.1004739	9.9074699	8.6914725
C	-0.1621920	8.9821205	8.3920307
C	-4.3984366	6.5614954	9.6182260
H	-3.3492499	6.5652399	9.9438476
H	-4.8319024	5.5812380	9.8580495
H	-4.9487748	7.3327909	10.1749638
C	0.4822201	10.1215113	8.9311308
H	-0.1341338	10.9600161	9.2602247
C	-3.6672831	1.3999874	5.2746145
H	-4.2790936	0.5825634	4.8959733
C	-4.2567717	2.5017632	5.8693315
H	-5.3434050	2.5520672	5.9588912
C	-3.7945179	8.1746453	7.7680856
H	-4.1716053	8.9672750	8.4370645
H	-4.0458815	8.4492399	6.7310208
C	2.6583108	9.1184787	8.6226121
H	3.7408572	9.1887732	8.7122121
C	-2.2688101	1.3300040	5.1550571
H	-1.8153127	0.4589521	4.6856937
C	1.8597365	10.1951966	9.0443189
H	2.3337433	11.0838231	9.4586013
C	4.1795741	6.9058816	7.7287582
H	4.5778929	7.7314246	7.1204400
H	4.5496173	5.9526693	7.3293475
H	4.5124110	7.0136625	8.7717225
C	-5.9472568	6.8868453	7.6478093
H	-6.4270308	7.7818249	8.0670585
H	-6.5246492	6.0217032	8.0000926
H	-6.0230645	6.9394571	6.5523899
C	0.5552793	1.2784612	4.9743587
H	0.3331407	0.3568014	5.5326315
H	1.6343441	1.4754634	5.0202438
H	0.2538986	1.1625952	3.9226197
Ba	1.1716655	4.7152885	6.6448700

Ni (II) L^{en}

Ni	-1.8520921	6.3073483	7.3755024
O	-0.0328148	6.7035110	7.4439609
O	-1.2802841	4.6643113	6.7229365
O	-0.0004214	2.6381303	5.6836231
O	2.5768101	6.6868395	7.5201063
N	-3.6501447	5.8553553	7.3893260
N	-2.3711617	7.9773581	7.9471704
C	-2.0198935	3.6896767	6.2947991
C	0.5231755	7.7679570	7.9335249
C	-1.3598631	2.5429457	5.7147993
C	-4.5086276	6.8477807	8.1063494
C	-4.1639176	4.7349354	6.9508746
H	-5.2472209	4.5980152	7.0453156
C	1.9661557	7.8095725	7.9939486
C	-3.4497997	3.6538209	6.3647111
C	-1.6015974	8.9530794	8.3558350
H	-2.0941304	9.8838336	8.6695286
C	-0.1821372	8.9194521	8.4145127
C	-4.4668436	6.5157318	9.6073863
H	-3.4299661	6.5226809	9.9691661
H	-4.8858211	5.5158369	9.7839032
H	-5.0520079	7.2482799	10.1820146
C	0.5226819	10.0448344	8.9273822
H	-0.0470429	10.9064814	9.2813910

C	-3.5122094	1.4573748	5.3254685
H	-4.0631546	0.5957142	4.9488494
C	-4.1741957	2.5293559	5.8768345
H	-5.2639705	2.5342882	5.9465518
C	-3.8131220	8.1850672	7.8301368
H	-4.1648105	8.9671389	8.5224290
H	-4.0408924	8.5012646	6.7985057
C	2.6193314	8.9220096	8.5037902
H	3.7075691	8.9405940	8.5462620
C	-2.0985456	1.4667865	5.2459339
H	-1.5901659	0.6089127	4.8077167
C	1.8973165	10.0461008	8.9726511
H	2.4409793	10.9054332	9.3647668
C	3.9988434	6.6500016	7.5507151
H	4.4402893	7.4501337	6.9308478
H	4.2799669	5.6744048	7.1387490
H	4.3867249	6.7367053	8.5810642
C	-5.9532857	6.9048047	7.5988280
H	-6.4548977	7.7814627	8.0318634
H	-6.5336513	6.0223993	7.8991017
H	-5.9855404	6.9933637	6.5039054
C	0.7223589	1.5427806	5.1340382
H	0.5452926	0.6124265	5.7020909
H	1.7803847	1.8176015	5.2087278
H	0.4627536	1.3732183	4.0740598

Ni (II)L^{en} + Li⁺

Ni	-1.9280494	6.3442833	7.4085826
O	-0.1069050	6.7030384	7.3937380
O	-1.2964506	4.7024905	6.8258802
O	0.0739693	2.8040533	5.7833516
O	2.4479632	6.5455350	7.4540084
N	-3.7050272	5.8718903	7.4180673
N	-2.4238614	8.0139793	7.9641828
C	-2.0143887	3.7066276	6.3481372
C	0.4946356	7.7627563	7.8955215
C	-1.2975453	2.6249244	5.7695112
C	-4.5697995	6.8717334	8.1321499
C	-4.1836384	4.7421287	6.9739080
H	-5.2650448	4.5831460	7.0488115
C	1.9144315	7.7257514	7.9387086
C	-3.4307577	3.6654749	6.3931132
C	-1.6239279	8.9741279	8.3408359
H	-2.0851304	9.9200890	8.6528385
C	-0.1906316	8.9090897	8.3750469
C	-4.5258543	6.5359629	9.6319685
H	-3.4916886	6.5445078	10.0022386
H	-4.9478839	5.5383946	9.8109314
H	-5.1128457	7.2691496	10.2018183
C	0.5626946	10.0029896	8.8760423
H	0.0384802	10.8877761	9.2396966
C	-3.3885696	1.4876210	5.3118881
H	-3.9081153	0.6204879	4.9068771
C	-4.1027029	2.5302877	5.8688579
H	-5.1922319	2.4924678	5.9069836
C	-3.8739023	8.2154971	7.8592949
H	-4.2225115	8.9906102	8.5579668
H	-4.0984912	8.5409714	6.8312454
C	2.6273340	8.8066632	8.4368278
H	3.7152980	8.7880699	8.4726799
C	-1.9783382	1.5299503	5.2572816
H	-1.4386432	0.6970879	4.8092604
C	1.9423389	9.9490667	8.9048777
H	2.5170778	10.7895041	9.2911631
C	3.8817986	6.4250095	7.4736752
H	4.3500677	7.2004258	6.8485576
H	4.1094207	5.4367673	7.0602879
H	4.2667782	6.4892449	8.5029289
C	-6.0096611	6.9154405	7.6151382
H	-6.5231156	7.7845956	8.0476959
H	-6.5820601	6.0280662	7.9150817
H	-6.0401994	7.0070657	6.5207241
C	0.8715750	1.7496603	5.2150504
H	0.7196788	0.8052267	5.7596542
H	1.9144832	2.0667038	5.3200994
H	0.6363515	1.6107203	4.1487688
Li	0.5819960	5.0299883	6.7903441

Ni (II)L^{en} + Na⁺

Ni	-1.8923800	6.3244008	7.3995150
O	-0.0631553	6.7084887	7.4324789
O	-1.2936978	4.6720969	6.7742085
O	0.0250658	2.6707448	5.7247209
O	2.5515719	6.6476764	7.5011259
N	-3.6782669	5.8637273	7.4081325
N	-2.3999871	7.9939767	7.9603743
C	-2.0301571	3.6828338	6.3170182
C	0.5169795	7.7806488	7.9268556
C	-1.3580826	2.5638613	5.7402428
C	-4.5435684	6.8614063	8.1234649
C	-4.1773722	4.7453451	6.9609458
H	-5.2604475	4.6040270	7.0426103
C	1.9432425	7.7995749	7.9790796
C	-3.4503341	3.6599388	6.3747164
C	-1.6188790	8.9620507	8.3531399
H	-2.0981201	9.8995136	8.6636818
C	-0.1893695	8.9210186	8.4022446
C	-4.4988886	6.5249614	9.6229668
H	-3.4638896	6.5319037	9.9909604
H	-4.9208127	5.5268575	9.8000419
H	-5.0845601	7.2573975	10.1953987
C	0.5259725	10.0379597	8.9063282
H	-0.0302552	10.9065029	9.2620671
C	-3.4862313	1.4737975	5.3133866
H	-4.0314829	0.6160772	4.9224257
C	-4.1610129	2.5409003	5.8687408
H	-5.2506219	2.5370301	5.9229525
C	-3.8479465	8.1995027	7.8461898
H	-4.1971669	8.9800664	8.5386003
H	-4.0679739	8.5186176	6.8150086
C	2.6177445	8.9031416	8.4799868
H	3.7055068	8.9156957	8.5199875
C	-2.0769275	1.4843410	5.2483130
H	-1.5635950	0.6321575	4.8063945
C	1.9046427	10.0280393	8.9451468
H	2.4542404	10.8846155	9.3326300
C	3.9890942	6.6092305	7.5470606
H	4.4266665	7.4076621	6.9287247
H	4.2829346	5.6352117	7.1396246
H	4.3536125	6.6942820	8.5822125
C	-5.9840916	6.9085209	7.6072146
H	-6.4924425	7.7822767	8.0366009
H	-6.5618215	6.0256334	7.9101901
H	-6.0143482	6.9970472	6.5123628
C	0.7520094	1.5749589	5.1421699
H	0.5673742	0.6402098	5.6933920
H	1.8138174	1.8350640	5.2192260
H	0.4860863	1.4437914	4.0820610
Na	0.9797246	4.8223160	6.6893780

Ni (II)L^{en} + K⁺

Ni	-1.8315826	6.2893282	7.3681977
O	0.0152816	6.7109959	7.4631674
O	-1.2715568	4.6108321	6.7016899
O	-0.0563344	2.4928506	5.6020555
O	2.6831818	6.7911753	7.6056463
N	-3.6296818	5.8395532	7.4047753
N	-2.3618928	7.9693609	7.8986652
C	-2.0421909	3.6337063	6.2663745
C	0.5565707	7.8037965	7.9653734
C	-1.4405151	2.4771868	5.6702630
C	-4.4893948	6.8476145	8.1121796
C	-4.1543470	4.7320678	6.9662872
H	-5.2374389	4.6087146	7.0700284
C	1.9838393	7.8959520	8.0636572
C	-3.4644548	3.6388410	6.3620808
C	-1.6113423	8.9476246	8.3176472
H	-2.1173352	9.8766888	8.6105947
C	-0.1895306	8.9328881	8.4169159
C	-4.4072679	6.5625398	9.6203177
H	-3.3647334	6.5873822	9.9644847
H	-4.8190086	5.5688908	9.8409267
H	-4.9847998	7.3106517	10.1806754
C	0.4607639	10.0779773	8.9446155

H	-0.1462350	10.9214920	9.2768035
C	-3.6216460	1.4574058	5.3051210
H	-4.2071699	0.6193731	4.9304146
C	-4.2338598	2.5477792	5.8817973
H	-5.3201994	2.5881614	5.9749428
C	-3.8072129	8.1708827	7.7678467
H	-4.1566345	8.9854288	8.4197656
H	-4.0274252	8.4346077	6.7212654
C	2.5949412	9.0273503	8.5869571
H	3.6796488	9.0802779	8.6584760
C	-2.2175706	1.4263312	5.2022495
H	-1.7459809	0.5574257	4.7473883
C	1.8341435	10.1254983	9.0328760
H	2.3387139	11.0008817	9.4385747
C	4.1166706	6.8553388	7.6723384
H	4.5071411	7.6804194	7.0566879
H	4.4873133	5.9033816	7.2734946
H	4.4634160	6.9676930	8.7112307
C	-5.9440003	6.8734659	7.6348834
H	-6.4403190	7.7606406	8.0509489
H	-6.5116980	6.0012186	7.9840359
H	-6.0081481	6.9275858	6.5391628
C	0.5781646	1.3407070	5.0230231
H	0.3507887	0.4297296	5.5980987
H	1.6575505	1.5303000	5.0642262
H	0.2780517	1.2044232	3.9725013
K	1.3837258	4.6126818	6.5705704

Ni (II)L^{en} + Mg²⁺

Ni	-2.0181902	6.3787872	7.4273415
O	-0.2532403	6.8000219	7.0564545
O	-1.3294813	4.6742242	7.2144185
O	0.1976485	3.1189777	5.9212100
O	2.2043742	6.2872387	7.3506829
N	-3.7713876	5.8557454	7.5248585
N	-2.5023111	8.0827917	7.8637128
C	-1.9888742	3.7112005	6.5651157
C	0.4099042	7.7711335	7.6883098
C	-1.1904623	2.7862041	5.8793766
C	-4.6332654	6.9021901	8.1832228
C	-4.2088124	4.6976202	7.1180174
H	-5.2850482	4.5027913	7.1820398
C	1.7881552	7.5641723	7.8314648
C	-3.3961161	3.6398706	6.5375227
C	-1.6739428	9.0381965	8.1812577
H	-2.0983758	10.0059282	8.4768148
C	-0.2263745	8.9162356	8.2101371
C	-4.5408464	6.6750695	9.7010825
H	-3.4987575	6.7238830	10.0462604
H	-4.9476895	5.6906759	9.9659396
H	-5.1229748	7.4425641	10.2279317
C	0.6001734	9.9037938	8.7951781
H	0.1526004	10.8138858	9.1964807
C	-3.1705258	1.5848725	5.2496547
H	-3.6281307	0.7368431	4.7419494
C	-3.9732083	2.5294996	5.8783684
H	-5.0582930	2.4247099	5.8477601
C	-3.9632707	8.2431182	7.7931289
H	-4.3102808	9.0589026	8.4431228
H	-4.2166142	8.4910790	6.7511325
C	2.5882879	8.5322572	8.4184865
H	3.6634810	8.4054063	8.5358196
C	-1.7660723	1.7088941	5.2239493
H	-1.1724977	0.9704343	4.6880445
C	1.9744513	9.7138333	8.8830563
H	2.5992100	10.4807905	9.3388030
C	3.6448056	6.0277094	7.3629707
H	4.1581649	6.7835443	6.7559573
H	3.7811037	5.0367662	6.9164193
H	4.0157202	6.0277669	8.3956702
C	-6.0815799	6.8797758	7.6948711
H	-6.6093050	7.7603441	8.0839230
H	-6.6233449	6.0003516	8.0655186
H	-6.1390887	6.9041548	6.5978068
C	1.1164084	2.1461697	5.3259332
H	0.9997011	1.1783635	5.8293712
H	2.1253394	2.5366554	5.4973840

H	0.9246695	2.0619505	4.2487689
Mg	0.5625636	5.0297055	6.7995986

Ni (II)L^{en} + Ca²⁺

Ni	-1.9294919	6.3427171	7.4107687
O	-0.0914223	6.7191386	7.3833615
O	-1.2984199	4.6775837	6.8320032
O	0.0632062	2.7663131	5.7620540
O	2.4819044	6.5700143	7.4726517
N	-3.7075571	5.8689901	7.4257357
N	-2.4272693	8.0171827	7.9576766
C	-2.0348368	3.6744723	6.3403644
C	0.5120662	7.7945306	7.9030140
C	-1.3369301	2.5987848	5.7589457
C	-4.5763376	6.8766481	8.1389351
C	-4.1896428	4.7468398	6.9775923
H	-5.2724039	4.5972815	7.0507191
C	1.9188691	7.7675106	7.9598648
C	-3.4453013	3.6579448	6.3915787
C	-1.6328683	8.9777751	8.3336497
H	-2.0977892	9.9229183	8.6414544
C	-0.1924289	8.9240934	8.3763228
C	-4.5244040	6.5438533	9.6388867
H	-3.4909732	6.5535132	10.0120509
H	-4.9497698	5.5490531	9.8240706
H	-5.1102441	7.2799105	10.2053821
C	0.5477121	10.0183177	8.8851109
H	0.0170942	10.8990995	9.2482245
C	-3.4239067	1.4810427	5.3034221
H	-3.9557511	0.6215270	4.8987779
C	-4.1265741	2.5345248	5.8649596
H	-5.2160522	2.5055455	5.9018415
C	-3.8819871	8.2156285	7.8504054
H	-4.2270457	8.9984672	8.5406173
H	-4.0999536	8.5319364	6.8186199
C	2.6312339	8.8464116	8.4644230
H	3.7187124	8.8379949	8.5121936
C	-2.0181408	1.5052165	5.2433075
H	-1.4902817	0.6666070	4.7926291
C	1.9316935	9.9767781	8.9261760
H	2.4936126	10.8218238	9.3205413
C	3.9363438	6.4815744	7.4976075
H	4.3763814	7.2661407	6.8682275
H	4.1919386	5.4974067	7.0867780
H	4.3046392	6.5539466	8.5294061
C	-6.0159116	6.9110171	7.6216953
H	-6.5301884	7.7811012	8.0510292
H	-6.5869946	6.0265435	7.9322363
H	-6.0515449	6.9992939	6.5271032
C	0.8463316	1.6826302	5.1829528
H	0.6777214	0.7517863	5.7402492
H	1.8981761	1.9781951	5.2763188
H	0.5944115	1.5553758	4.1218940
Ca	0.8987749	4.8640981	6.7084693

Ni (II)L^{en} + Ba²⁺

Ni	-1.8446542	6.2923659	7.3796326
O	0.0207650	6.7065146	7.4535864
O	-1.2632234	4.5978628	6.7275463
O	-0.0456850	2.5108033	5.6203049
O	2.6695186	6.7681663	7.6052568
N	-3.6390704	5.8398366	7.4141868
N	-2.3717283	7.9754452	7.8994105
C	-2.0501970	3.6092956	6.2680745
C	0.5720070	7.8209659	7.9659061
C	-1.4458834	2.4754853	5.6737390
C	-4.5028196	6.8537162	8.1229823
C	-4.1561249	4.7359692	6.9685455
H	-5.2399862	4.6139817	7.0658351
C	1.9821843	7.9002724	8.0639048
C	-3.4624963	3.6361743	6.3610156
C	-1.6153980	8.9494599	8.3079213
H	-2.1154814	9.8828588	8.5954745
C	-0.1853916	8.9345998	8.4061037
C	-4.4128463	6.5689812	9.6304059
H	-3.3714822	6.5965871	9.9787150
H	-4.8268385	5.5777482	9.8558689

H	-4.9906553	7.3182101	10.1878966
C	0.4679924	10.0762868	8.9293152
H	-0.1319185	10.9245737	9.2607452
C	-3.6090269	1.4596937	5.2867147
H	-4.1970040	0.6268983	4.9047769
C	-4.2260142	2.5512586	5.8673928
H	-5.3128375	2.5877653	5.9492584
C	-3.8220347	8.1747871	7.7686685
H	-4.1672116	8.9926604	8.4166965
H	-4.0358968	8.4355941	6.7207015
C	2.6091015	9.0270434	8.5820392
H	3.6937752	9.0777756	8.6548999
C	-2.2093818	1.4201837	5.1896052
H	-1.7363287	0.5534606	4.7322602
C	1.8460502	10.1212801	9.0191460
H	2.3481832	10.9984411	9.4235807
C	4.1202755	6.8148905	7.6628961
H	4.5049445	7.6309545	7.0365592
H	4.4766719	5.8556862	7.2664587
H	4.4631790	6.9250636	8.7004134
C	-5.9565240	6.8671462	7.6457057
H	-6.4581184	7.7498845	8.0639563
H	-6.5175881	5.9930090	8.0006734
H	-6.0265339	6.9231013	6.5505379
C	0.6166403	1.3614424	5.0283270
H	0.3938174	0.4505974	5.6002831
H	1.6937853	1.5652208	5.0796887
H	0.3220298	1.2432463	3.9768416
Ba	1.2538601	4.6638540	6.6418444

Ni (I) L^{pn}

Ni	4.6788985	0.2599937	6.4426565
O	5.9039854	-0.4498302	5.0290233
O	4.5019696	1.7410766	5.1013331
O	7.6101970	-0.6464179	3.0174687
O	5.0281009	3.4710905	3.1694768
N	5.0754671	-1.2902316	7.5752000
N	3.4882869	1.2316198	7.6638340
C	4.1693457	2.9562668	5.3160229
C	6.8401433	-1.3103389	5.1564516
C	7.8182258	-1.4768353	4.0931840
C	7.0122128	-2.1580306	6.3119815
C	6.1106847	-2.0884272	7.4163353
H	6.3269515	-2.8008016	8.2348726
C	3.5403345	3.4236822	6.5286839
C	4.4240898	3.9663982	4.3011974
C	8.8489668	-2.3989784	4.1866636
H	9.5678334	-2.5064296	3.3732776
C	2.9572967	0.5845106	8.8579956
H	2.1046405	-0.0545552	8.5605984
H	2.5606163	1.3476957	9.5607183
C	3.2367283	2.5222208	7.5931039
H	2.7295355	2.9847230	8.4612329
C	3.9643067	-0.2980973	9.6202891
C	8.0841692	-3.0898875	6.3719771
H	8.1788615	-3.7153929	7.2653569
C	4.3051853	-1.5485471	8.7873595
H	4.8491108	-2.2646129	9.4394294
H	3.3531930	-2.0342945	8.5002780
C	8.9881928	-3.2156948	5.3379131
H	9.8064190	-3.9356273	5.3931184
C	5.2334661	0.4940291	9.9553763
H	5.7267604	0.8268740	9.0316083
H	5.9420271	-0.1283880	10.5236172
H	4.9886028	1.3831031	10.5573190
C	4.0729906	5.2947948	4.4870494
H	4.2698094	6.0310132	3.7067923
C	3.1994505	4.7952902	6.6843059
H	2.7216163	5.1092898	7.6177766
C	3.4553018	5.7186053	5.6917134
H	3.1862749	6.7683574	5.8199124
C	3.2781484	-0.7738272	10.9116377
H	3.0040155	0.0818069	11.5478084
H	3.9468302	-1.4266152	11.4932682
H	2.3587394	-1.3402444	10.6910883
C	8.5374375	-0.7187150	1.9544860
H	9.5652570	-0.4702030	2.2827808

H	8.2074165	0.0211055	1.2140318
H	8.5548621	-1.7205314	1.4826923
C	5.3420112	4.3931081	2.1463045
H	4.4379809	4.8791440	1.7307188
H	5.8333287	3.8119541	1.3554217
H	6.0325551	5.1841170	2.4973794

Ni (I) L^{pn} + Li⁺

Ni	4.3857970	0.0761614	6.4792675
O	5.5095646	-0.6384333	4.9422793
O	4.2065983	1.4875086	5.0261348
O	7.2710364	-0.3252685	3.0814145
O	5.2084677	3.0360183	3.2236080
N	4.9353483	-1.3999942	7.5970707
N	3.3342271	1.1538741	7.6877310
C	4.0708387	2.7608058	5.2615639
C	6.6028913	-1.3275512	5.1008843
C	7.6036493	-1.2393391	4.0855176
C	6.8754914	-2.1283368	6.2499733
C	6.0036421	-2.1353973	7.3980741
H	6.3110945	-2.8150575	8.2106430
C	3.4989697	3.2900725	6.4570208
C	4.5621591	3.6780245	4.2832289
C	8.7696590	-1.9845039	4.1425164
H	9.5184930	-1.9250481	3.3533988
C	2.8758469	0.5467563	8.9367099
H	2.0081992	-0.0946471	8.7037232
H	2.5291925	1.3316583	9.6367966
C	3.1373217	2.4453271	7.5676324
H	2.6807656	2.9718273	8.4232380
C	3.9359885	-0.3172604	9.6592149
C	8.0741306	-2.8858617	6.2841566
H	8.2722951	-3.5129243	7.1567651
C	4.2389351	-1.6102057	8.8664593
H	4.8268298	-2.2878435	9.5159907
H	3.2806579	-2.1138950	8.6480977
C	8.9951330	-2.8296836	5.2527928
H	9.9095724	-3.4207022	5.2957458
C	5.2204217	0.4876271	9.8923324
H	5.6668160	0.7927479	8.9358648
H	5.9606475	-0.1120148	10.4426334
H	5.0095420	1.3952935	10.4776435
C	4.4070361	5.0474025	4.4228634
H	4.7689906	5.7393810	3.6630366
C	3.3446338	4.6950985	6.5749505
H	2.8873594	5.0966618	7.4824122
C	3.7746579	5.5560474	5.5804056
H	3.6463848	6.6327074	5.6884538
C	3.3268869	-0.7457544	11.0058478
H	3.0862086	0.1319810	11.6234220
H	4.0321488	-1.3706339	11.5729584
H	2.4004193	-1.3237912	10.8639871
C	8.2199111	-0.1532022	2.0276207
H	9.1868087	0.2081482	2.4151418
H	7.7954030	0.5969736	1.3495958
H	8.3760341	-1.0941066	1.4750615
C	5.7555256	3.8727723	2.2036555
H	4.9670527	4.4584470	1.7036732
H	6.2256179	3.2029255	1.4736367
H	6.5151942	4.5586233	2.6142320
Li	5.4477031	0.8368843	3.7610213

Ni (I) L^{pn} + Na⁺

Ni	4.7297112	0.2903236	6.5332718
O	5.9863896	-0.3962884	5.0852877
O	4.6193273	1.7972595	5.1678117
O	7.6975641	-0.5699225	3.0791489
O	5.1358616	3.5120009	3.2194694
N	5.1119463	-1.2857749	7.6113184
N	3.5280717	1.2715528	7.7102501
C	4.1819897	3.0081590	5.3367996
C	6.8803909	-1.3339514	5.1738602
C	7.8393199	-1.4951565	4.1174765
C	6.9780047	-2.2267644	6.2858081
C	6.0837365	-2.1419009	7.4078133
H	6.2564589	-2.9053917	8.1858445
C	3.4738629	3.4326822	6.5043265

C	4.4185573	3.9942626	4.3197249
C	8.8086857	-2.4848466	4.1513318
H	9.5255016	-2.5973330	3.3385998
C	3.0029674	0.6172593	8.9110395
H	2.1472764	-0.0113931	8.6062363
H	2.6142377	1.3779392	9.6157732
C	3.1927076	2.5332508	7.5901983
H	2.6179238	2.9845379	8.4174489
C	4.0101909	-0.2758522	9.6601350
C	7.9806914	-3.2285975	6.2960335
H	8.0339885	-3.9036399	7.1537142
C	4.3339612	-1.5317058	8.8281939
H	4.8650072	-2.2562505	9.4760452
H	3.3796299	-2.0016119	8.5295471
C	8.8780554	-3.3638549	5.2538148
H	9.6419067	-4.1407079	5.2737512
C	5.2870602	0.5028674	10.0007461
H	5.7907559	0.8443214	9.0857330
H	5.9879936	-0.1299936	10.5652834
H	5.0498808	1.3857089	10.6132705
C	3.9691981	5.2994702	4.4435545
H	4.1530294	6.0330732	3.6595352
C	3.0277677	4.7745152	6.6066039
H	2.4850297	5.0765385	7.5056311
C	3.2634481	5.6933650	5.6012152
H	2.9123567	6.7208752	5.6920370
C	3.3216215	-0.7512389	10.9515323
H	3.0557746	0.1038244	11.5903219
H	3.9873676	-1.4078398	11.5304156
H	2.3986548	-1.3111155	10.7332644
C	8.6086158	-0.6873095	1.9868899
H	9.6521965	-0.5447979	2.3144427
H	8.3439766	0.1043846	1.2747612
H	8.5147920	-1.6664618	1.4886554
C	5.3778590	4.4349213	2.1573912
H	4.4341881	4.8069458	1.7254949
H	5.9326445	3.8835823	1.3875027
H	5.9845632	5.2910761	2.4967323
Na	5.9615011	1.1713034	3.5270112

Ni (I) L^{Pn} + K⁺

Ni	4.6730235	0.2598653	6.4574589
O	5.9068309	-0.4989959	4.9940599
O	4.4772202	1.7773545	5.0755625
O	7.6411110	-0.7690073	2.9741152
O	4.9113517	3.5512083	3.1188501
N	5.0803627	-1.2881680	7.5762385
N	3.5200345	1.2539448	7.6802470
C	4.1522801	3.0123328	5.3141467
C	6.8712300	-1.3556807	5.1534451
C	7.8471951	-1.5495587	4.1123563
C	7.0365868	-2.1498945	6.3343368
C	6.1159290	-2.0775771	7.4323536
H	6.3235215	-2.7921489	8.2475760
C	3.5771384	3.4530093	6.5508100
C	4.3617765	4.0251973	4.3117497
C	8.8967421	-2.4464582	4.2437410
H	9.6237022	-2.5750831	3.4426197
C	2.9728952	0.5983087	8.8695105
H	2.1152231	-0.0202839	8.5505764
H	2.5825907	1.3590873	9.5733909
C	3.2770920	2.5396057	7.6164935
H	2.7671204	3.0003504	8.4803842
C	3.9634399	-0.3057425	9.6246038
C	8.1181633	-3.0600944	6.4401372
H	8.2122232	-3.6506853	7.3548018
C	4.2886465	-1.5508863	8.7796082
H	4.8111992	-2.2865110	9.4221211
H	3.3361629	-2.0131605	8.4647217
C	9.0376767	-3.2102365	5.4213503
H	9.8665937	-3.9115361	5.5135645
C	5.2416596	0.4634168	9.9805622
H	5.7543965	0.8062781	9.0712615
H	5.9343682	-0.1761839	10.5476681
H	5.0045238	1.3445003	10.5956052
C	4.0373963	5.3559412	4.5284482
H	4.2065665	6.1033735	3.7543055

C	3.2551482	4.8201342	6.7442032
H	2.8166431	5.1207632	7.6990704
C	3.4797530	5.7615015	5.7593232
H	3.2290003	6.8098814	5.9187375
C	3.2601758	-0.7891380	10.9043347
H	2.9918093	0.0613265	11.5482828
H	3.9170882	-1.4539750	11.4839521
H	2.3369875	-1.3429020	10.6716402
C	8.6202422	-0.8685101	1.9430942
H	9.6220189	-0.5854880	2.3077127
H	8.3156871	-0.1667804	1.1556485
H	8.6642797	-1.8863803	1.5192494
C	5.2062162	4.5215459	2.1173429
H	4.2941876	5.0295977	1.7602808
H	5.6623726	3.9770400	1.2801174
H	5.9207505	5.2773208	2.4846893
K	5.3178650	0.7944809	2.8716380

Ni (I) L^{pn} + Mg²⁺

Ni	4.2712349	0.0059022	6.4853889
O	5.3400604	-0.7702037	4.9049439
O	3.9912780	1.3922212	4.9858797
O	7.1020315	-0.1709016	3.1150520
O	5.2584416	2.8071552	3.2359159
N	4.8995438	-1.4315713	7.6012474
N	3.2883121	1.1373231	7.6939803
C	4.0227597	2.6948250	5.2456308
C	6.5292454	-1.3323746	5.0906184
C	7.5220682	-1.1068213	4.1132850
C	6.8560965	-2.0819427	6.2463149
C	5.9770724	-2.1423956	7.4003325
H	6.3040884	-2.8229395	8.2014051
C	3.5301846	3.2531511	6.4499378
C	4.6364277	3.5397658	4.2963144
C	8.7712532	-1.7009996	4.1732705
H	9.5280842	-1.5382565	3.4079083
C	2.8323058	0.5267420	8.9466782
H	1.9633916	-0.1077895	8.7063461
H	2.4907874	1.3100952	9.6469363
C	3.1203390	2.4268632	7.5710147
H	2.6768924	2.9735937	8.4178018
C	3.8974422	-0.3414620	9.6601215
C	8.1258698	-2.7020521	6.2918878
H	8.3852060	-3.3068187	7.1625771
C	4.1977209	-1.6399279	8.8723530
H	4.7821058	-2.3173220	9.5209245
H	3.2430813	-2.1419654	8.6422202
C	9.0544480	-2.5339919	5.2728779
H	10.0253885	-3.0233932	5.3299643
C	5.1837346	0.4619167	9.8900472
H	5.6340231	0.7716661	8.9363808
H	5.9230697	-0.1379157	10.4398526
H	4.9760611	1.3665622	10.4797773
C	4.6593958	4.9172983	4.4340907
H	5.1181122	5.5671807	3.6907492
C	3.5387112	4.6612379	6.5752979
H	3.1370965	5.1107240	7.4851613
C	4.0708638	5.4764112	5.5848330
H	4.0641526	6.5587158	5.7032914
C	3.2902587	-0.7697733	11.0085744
H	3.0537728	0.1082329	11.6259926
H	3.9974520	-1.3926145	11.5739723
H	2.3636146	-1.3471518	10.8710889
C	8.0115620	0.0646395	2.0138626
H	8.9433720	0.5184115	2.3773348
H	7.5003584	0.7549635	1.3338229
H	8.2191292	-0.8788303	1.4921858
C	5.8403759	3.5812701	2.1601181
H	5.0727283	4.2160838	1.6986700
H	6.2093019	2.8583154	1.4243717
H	6.6729309	4.1919407	2.5351527
Mg	5.3509612	0.7825063	3.7543420

Ni (I) L^{pn} + Ca²⁺

Ni	4.6839230	0.2589353	6.5724282
O	5.9422243	-0.4081093	5.0689950
O	4.5845750	1.7609645	5.1512546

O	7.6345949	-0.5067385	3.0932768
O	5.1919096	3.4378230	3.2483229
N	5.1124277	-1.3020987	7.6312038
N	3.4976678	1.2659596	7.7230723
C	4.1580152	3.0037609	5.3308200
C	6.8718885	-1.3487472	5.1656280
C	7.8162630	-1.4676861	4.1182101
C	6.9701427	-2.2241321	6.2752836
C	6.0778646	-2.1545427	7.4125587
H	6.2589378	-2.9265967	8.1766882
C	3.4507816	3.4141209	6.4884323
C	4.4407302	3.9638914	4.3295971
C	8.8136324	-2.4299074	4.1285430
H	9.5338673	-2.5176819	3.3168134
C	2.9818972	0.6045651	8.9298297
H	2.1347668	-0.0298671	8.6184293
H	2.5861570	1.3613577	9.6308158
C	3.1525501	2.5182947	7.5858073
H	2.5630848	2.9763660	8.3957844
C	4.0039121	-0.2769003	9.6761948
C	7.9916381	-3.2032580	6.2712563
H	8.0660726	-3.8854566	7.1200255
C	4.3368238	-1.5406267	8.8571340
H	4.8751723	-2.2534130	9.5074841
H	3.3902295	-2.0217215	8.5564574
C	8.8911711	-3.3106005	5.2229285
H	9.6688990	-4.0725729	5.2398422
C	5.2742648	0.5153720	10.0116912
H	5.7813251	0.8605798	9.0996145
H	5.9797018	-0.1064839	10.5811930
H	5.0302081	1.3974138	10.6213311
C	4.0221982	5.2816459	4.4297857
H	4.2396728	6.0127079	3.6530780
C	3.0269278	4.7615153	6.5761876
H	2.4744886	5.0802336	7.4618583
C	3.2995566	5.6758150	5.5709942
H	2.9634780	6.7078617	5.6585550
C	3.3212980	-0.7520857	10.9721633
H	3.0533894	0.1033969	11.6082101
H	3.9940511	-1.3993609	11.5519860
H	2.4020357	-1.3196334	10.7619004
C	8.5345338	-0.5861502	1.9670946
H	9.5735524	-0.4221956	2.2870165
H	8.2378131	0.2111227	1.2738664
H	8.4404332	-1.5588821	1.4639809
C	5.5020581	4.3509836	2.1735299
H	4.5807490	4.7311262	1.7104160
H	6.0708820	3.7762528	1.4313899
H	6.1176849	5.1858724	2.5373168
Ca	5.8520769	1.1038103	3.5318234

Ni (I) L^{Pn} + Ba²⁺

Ni	4.6136084	0.2195059	6.4855534
O	5.8316374	-0.5379817	4.9672591
O	4.4140826	1.7292397	5.0534094
O	7.5447606	-0.7289784	2.9679730
O	4.9351470	3.4593474	3.1258699
N	5.0726004	-1.3073004	7.5927178
N	3.4838573	1.2422186	7.6887283
C	4.1263558	3.0000966	5.3071807
C	6.8496919	-1.3728230	5.1409951
C	7.8102456	-1.5155969	4.1056449
C	7.0292112	-2.1351664	6.3247645
C	6.1098691	-2.0838845	7.4375317
H	6.3323307	-2.8027239	8.2418048
C	3.5694199	3.4319946	6.5396119
C	4.3869134	3.9812327	4.3146025
C	8.9024922	-2.3629718	4.2235223
H	9.6338504	-2.4592121	3.4228303
C	2.9450094	0.5807627	8.8836209
H	2.0956692	-0.0437403	8.5590170
H	2.5485079	1.3384227	9.5833753
C	3.2465412	2.5232889	7.6152686
H	2.7316250	2.9951571	8.4672387
C	3.9503104	-0.3109480	9.6370029
C	8.1434162	-3.0016928	6.4243153
H	8.2686438	-3.5886373	7.3359865

C	4.2844920	-1.5640815	8.8051653
H	4.8154107	-2.2873855	9.4503600
H	3.3398843	-2.0382923	8.4888823
C	9.0668257	-3.1145458	5.3998814
H	9.9210691	-3.7833491	5.4942251
C	5.2221345	0.4722709	9.9868172
H	5.7357880	0.8218163	9.0802859
H	5.9214583	-0.1570449	10.5557401
H	4.9786420	1.3506796	10.6019338
C	4.1176385	5.3270876	4.5178827
H	4.3258774	6.0682656	3.7483682
C	3.2940875	4.8072563	6.7273549
H	2.8604376	5.1286493	7.6760612
C	3.5635974	5.7408063	5.7417598
H	3.3484981	6.7959120	5.9036558
C	3.2527435	-0.7928097	10.9215589
H	2.9822842	0.0592131	11.5612271
H	3.9162437	-1.4480301	11.5031589
H	2.3329136	-1.3539470	10.6968888
C	8.5264060	-0.7633210	1.9152542
H	9.5060404	-0.4230215	2.2812152
H	8.1730509	-0.0750115	1.1365055
H	8.6131874	-1.7740454	1.4900134
C	5.3168662	4.4136951	2.1170011
H	4.4416773	4.9650336	1.7433385
H	5.7568329	3.8368752	1.2927719
H	6.0675866	5.1166528	2.5068828
Ba	5.1967289	0.7173620	2.9880855

Ni (II) L^{pn}

Ni	4.7411796	0.2982042	6.4697622
O	5.8397081	-0.3951492	5.1050386
O	4.5434337	1.6587614	5.1786288
O	7.3909468	-0.6244337	2.9970888
O	4.9638739	3.2724840	3.1463142
N	5.1587456	-1.1636049	7.6225523
N	3.6403405	1.2466278	7.7053173
C	4.3047342	2.9142136	5.3825291
C	6.8590560	-1.1824875	5.2256691
C	7.7484064	-1.3409664	4.0996089
C	7.1529599	-1.9312432	6.4047766
C	6.2262540	-1.9170969	7.4791957
H	6.4071725	-2.6588529	8.2692414
C	3.8077208	3.4419619	6.6125679
C	4.5243720	3.8459910	4.3020318
C	8.8639620	-2.1589150	4.2009623
H	9.5428960	-2.2574960	3.3546819
C	2.9470847	0.5566940	8.7962799
H	2.1259867	-0.0381243	8.3602841
H	2.4868976	1.3061023	9.4628985
C	3.4351835	2.5429783	7.6458051
H	2.8705008	2.9849211	8.4783924
C	3.8445870	-0.3706380	9.6240815
C	8.3002765	-2.7703606	6.4706413
H	8.4954275	-3.3301865	7.3876729
C	4.2804249	-1.5410593	8.7346656
H	4.7902730	-2.2968663	9.3568897
H	3.3804672	-2.0206916	8.3127527
C	9.1460760	-2.8740157	5.3907141
H	10.0314506	-3.5079527	5.4354025
C	5.0621935	0.3884680	10.1664550
H	5.6695712	0.7913533	9.3451878
H	5.6972501	-0.2763106	10.7699331
H	4.7448963	1.2274205	10.8031944
C	4.3020621	5.2020068	4.4930359
H	4.4916728	5.9021223	3.6804828
C	3.5783474	4.8373482	6.7704787
H	3.1975192	5.2072640	7.7246813
C	3.8320901	5.7031669	5.7317284
H	3.6681910	6.7744348	5.8469462
C	3.0043127	-0.9391408	10.7778539
H	2.6489922	-0.1322135	11.4350926
H	3.6004537	-1.6310548	11.3901926
H	2.1246155	-1.4866293	10.4058082
C	8.2199465	-0.7342060	1.8459195
H	9.2454130	-0.3769659	2.0467373
H	7.7564553	-0.0971171	1.0844221

H	8.2662135	-1.7735138	1.4754824
C	5.1992719	4.1314233	2.0367559
H	4.2793572	4.6590195	1.7281762
H	5.5343591	3.4796188	1.2222633
H	5.9852497	4.8750219	2.2568477

Ni (II)L^{Pn} + Li⁺

Ni	4.5907844	0.2058446	6.5087102
O	5.5923569	-0.5023957	5.0946318
O	4.3383248	1.4888087	5.1682963
O	7.1942722	-0.3043137	3.0836431
O	5.1848524	2.9535450	3.2187005
N	5.0835557	-1.2174624	7.6561982
N	3.5603489	1.2052419	7.7433274
C	4.2233118	2.7858724	5.3536919
C	6.7064699	-1.1920019	5.2013989
C	7.6071693	-1.1524720	4.1051134
C	7.0331701	-1.9561663	6.3427639
C	6.1292778	-1.9788940	7.4536536
H	6.3379821	-2.7371212	8.2190819
C	3.7161910	3.3509777	6.5442592
C	4.6332143	3.6383916	4.2954551
C	8.7772999	-1.8955456	4.1324609
H	9.4749564	-1.8716909	3.2968195
C	2.9194268	0.5415661	8.8864024
H	2.0799319	-0.0580486	8.4966997
H	2.4936367	1.3082756	9.5535162
C	3.3278150	2.4873603	7.6193125
H	2.7585659	2.9626592	8.4287165
C	3.8577824	-0.3672607	9.6907197
C	8.2287425	-2.7171369	6.3505858
H	8.4740733	-3.3198946	7.2261587
C	4.2511827	-1.5651573	8.8165455
H	4.7866209	-2.3056469	9.4326434
H	3.3376394	-2.0526060	8.4372245
C	9.0808048	-2.6871010	5.2620256
H	10.0018178	-3.2679753	5.2683630
C	5.0986074	0.4017923	10.1634166
H	5.6784746	0.7893456	9.3144296
H	5.7555951	-0.2497378	10.7565806
H	4.8084937	1.2525481	10.7961303
C	4.4906779	5.0131385	4.4075324
H	4.8032935	5.6759944	3.6021000
C	3.5668809	4.7569299	6.6384366
H	3.1597935	5.1916870	7.5524563
C	3.9450909	5.5694495	5.5853350
H	3.8354631	6.6503272	5.6580403
C	3.0665676	-0.9066549	10.8939601
H	2.7487416	-0.0838169	11.5495069
H	3.6871093	-1.5872791	11.4931787
H	2.1675927	-1.4561474	10.5768754
C	8.0302150	-0.2424529	1.9116799
H	9.0290228	0.1451656	2.1630059
H	7.5335167	0.4445374	1.2182921
H	8.1160468	-1.2343173	1.4441118
C	5.5854250	3.7421243	2.0813383
H	4.7246464	4.2847949	1.6639608
H	5.9638919	3.0337274	1.3367494
H	6.3821079	4.4495073	2.3558862
Li	5.4953673	0.8759847	3.7279773

Ni (II)L^{Pn} + Na⁺

Ni	4.7180561	0.2825068	6.4883190
O	5.7784757	-0.4385118	5.1014261
O	4.4857098	1.6243298	5.1770727
O	7.3734301	-0.6052581	2.9879105
O	4.9787268	3.2494482	3.1346247
N	5.1493994	-1.1586182	7.6383065
N	3.6441564	1.2358839	7.7204204
C	4.2962728	2.9087958	5.3834129
C	6.8460814	-1.1947692	5.2252752
C	7.7370565	-1.3256733	4.1177331
C	7.1480027	-1.9111499	6.4100356
C	6.2167144	-1.9014301	7.4913607
H	6.4041802	-2.6444879	8.2769001
C	3.8306428	3.4290931	6.6170288
C	4.5414947	3.8282765	4.3194690

C	8.8745386	-2.1135989	4.2169680
H	9.5611413	-2.2008298	3.3766074
C	2.9416270	0.5476298	8.8120034
H	2.1232634	-0.0403518	8.3644101
H	2.4799842	1.3010408	9.4700324
C	3.4502573	2.5278413	7.6568491
H	2.8868905	2.9773038	8.4847118
C	3.8324866	-0.3785132	9.6440660
C	8.3101987	-2.7188979	6.4860657
H	8.5180913	-3.2668420	7.4063141
C	4.2694305	-1.5434945	8.7521724
H	4.7828041	-2.3008254	9.3663692
H	3.3763588	-2.0240564	8.3196694
C	9.1652669	-2.8111938	5.4075752
H	10.0643020	-3.4231918	5.4612431
C	5.0460866	0.3771203	10.2014456
H	5.6685662	0.7865134	9.3941621
H	5.6717372	-0.2902000	10.8107407
H	4.7231413	1.2110726	10.8407997
C	4.3558929	5.1904792	4.5072109
H	4.5594495	5.8916055	3.6999223
C	3.6362171	4.8229805	6.7834757
H	3.2706900	5.1988053	7.7402460
C	3.9050898	5.6915800	5.7457956
H	3.7671800	6.7646034	5.8689335
C	2.9799379	-0.9526785	10.7870849
H	2.6220154	-0.1485782	11.4451798
H	3.5706223	-1.6465246	11.4013000
H	2.1026423	-1.4973138	10.4068198
C	8.2181325	-0.7425290	1.8306536
H	9.2329234	-0.3680982	2.0343667
H	7.7589922	-0.1354969	1.0420274
H	8.2639958	-1.7910514	1.5001749
C	5.1700261	4.1315311	2.0134698
H	4.2341956	4.6519934	1.7595377
H	5.4694441	3.4966609	1.1717494
H	5.9651049	4.8645374	2.2174188
Na	5.4770755	0.8788316	3.2612324

Ni (II) L^{pn} + K⁺

Ni	4.6411528	0.2392624	6.4503754
O	5.6665792	-0.5230855	5.0587693
O	4.3393927	1.5642090	5.1348637
O	7.2757619	-0.7050176	2.9352437
O	4.8271935	3.2031170	3.0821540
N	5.1112685	-1.1632790	7.6273786
N	3.6238662	1.2101402	7.7133307
C	4.2744280	2.8567664	5.3678269
C	6.7935102	-1.1811195	5.2136871
C	7.6944794	-1.3063021	4.1099759
C	7.1576481	-1.8124640	6.4335051
C	6.2221576	-1.8427428	7.5102414
H	6.4465438	-2.5567062	8.3131641
C	3.9223218	3.3955295	6.6348205
C	4.5293745	3.7794477	4.3056793
C	8.8980161	-1.9832145	4.2554717
H	9.5912015	-2.0565859	3.4192732
C	2.9097672	0.5341385	8.8029114
H	2.0835178	-0.0423154	8.3549154
H	2.4582415	1.2936385	9.4616216
C	3.5081757	2.5113671	7.6760739
H	2.9929434	2.9825423	8.5232797
C	3.7895506	-0.4058600	9.6338501
C	8.3836519	-2.5137912	6.5516051
H	8.6319931	-2.9940702	7.4992972
C	4.2321528	-1.5642728	8.7336111
H	4.7468269	-2.3254816	9.3424687
H	3.3413133	-2.0438383	8.2955144
C	9.2490121	-2.5859079	5.4807111
H	10.1989026	-3.1114708	5.5657846
C	5.0019012	0.3406611	10.2058521
H	5.6303818	0.7562339	9.4065858
H	5.6220956	-0.3343725	10.8123694
H	4.6772797	1.1692082	10.8515140
C	4.4797002	5.1486573	4.5333148
H	4.6980414	5.8474286	3.7277413
C	3.8590464	4.7965047	6.8376759

H	3.5795214	5.1793500	7.8204033
C	4.1493960	5.6619175	5.8039568
H	4.1174330	6.7399665	5.9540245
C	2.9283397	-0.9867845	10.7661532
H	2.5685415	-0.1874347	11.4290442
H	3.5131966	-1.6878386	11.3778674
H	2.0519233	-1.5254420	10.3755793
C	8.1945877	-0.7313086	1.8322175
H	9.1396267	-0.2290638	2.0914805
H	7.7102060	-0.1839345	1.0150643
H	8.3990651	-1.7625093	1.5048499
C	5.1589428	4.0977605	2.0091952
H	4.3129972	4.7578243	1.7618332
H	5.3876932	3.4668106	1.1419479
H	6.0441660	4.7038856	2.2566793
K	4.6891721	0.4061464	2.7753451

Ni (II)L^{pn} + Mg²⁺

Ni	4.5337380	0.1685282	6.5211175
O	5.5033185	-0.5770073	5.0769539
O	4.2387930	1.4423809	5.1514354
O	7.1371626	-0.2044062	3.1079068
O	5.2511424	2.8574633	3.2347457
N	5.0593631	-1.2444083	7.6678224
N	3.5250252	1.1922079	7.7535389
C	4.1854863	2.7669964	5.3393450
C	6.6704334	-1.2224237	5.1858843
C	7.5761312	-1.1063320	4.1192018
C	7.0014586	-1.9751125	6.3229742
C	6.0959995	-2.0074339	7.4464890
H	6.3130737	-2.7707752	8.2035401
C	3.6892595	3.3303717	6.5250573
C	4.6647670	3.5890056	4.3066714
C	8.7781713	-1.7971801	4.1267056
H	9.4870967	-1.7257355	3.3035510
C	2.9003356	0.5289396	8.9108910
H	2.0603584	-0.0729137	8.5271460
H	2.4784746	1.2990831	9.5745789
C	3.2887804	2.4683563	7.6114881
H	2.7171106	2.9535944	8.4123373
C	3.8550470	-0.3682888	9.7096253
C	8.2220273	-2.6870484	6.3243735
H	8.4904126	-3.2953111	7.1888305
C	4.2369379	-1.5770416	8.8448135
H	4.7804605	-2.3105785	9.4599968
H	3.3233456	-2.0697445	8.4736006
C	9.0848694	-2.6044243	5.2390433
H	10.0238049	-3.1554556	5.2455410
C	5.0995474	0.4087890	10.1602227
H	5.6755457	0.7911752	9.3050470
H	5.7624774	-0.2330746	10.7562440
H	4.8148930	1.2645971	10.7877680
C	4.5819070	4.9700352	4.3985938
H	4.9405586	5.6215787	3.6032929
C	3.5946326	4.7372684	6.6121817
H	3.1919033	5.1953205	7.5162410
C	4.0245031	5.5366856	5.5608292
H	3.9495771	6.6203578	5.6335116
C	3.0780174	-0.8999783	10.9274359
H	2.7652811	-0.0719397	11.5780047
H	3.7097673	-1.5688521	11.5272925
H	2.1784008	-1.4577502	10.6288372
C	7.9640774	-0.0992712	1.9061458
H	8.9496599	0.3063051	2.1661563
H	7.4385384	0.5883724	1.2352592
H	8.0504765	-1.0849991	1.4334726
C	5.6794213	3.6223251	2.0639259
H	4.8211909	4.1608939	1.6446175
H	6.0458731	2.8878345	1.3390892
H	6.4855824	4.3116389	2.3431883
Mg	5.4799834	0.8636812	3.7355364

Ni (II)L^{pn} + Ca²⁺

Ni	4.6465057	0.2385477	6.4988170
O	5.6687431	-0.5067557	5.0731203
O	4.3642097	1.5561845	5.1489341
O	7.2825172	-0.5105703	2.9995369

O	5.0336243	3.1271715	3.1447705
N	5.1182280	-1.1829997	7.6561303
N	3.6011159	1.2145097	7.7369420
C	4.2506469	2.8741414	5.3643965
C	6.7983629	-1.2143637	5.2053985
C	7.6912300	-1.2680772	4.1167866
C	7.1090221	-1.9123927	6.3869697
C	6.1817386	-1.9193263	7.4852788
H	6.3863836	-2.6668885	8.2613155
C	3.8004091	3.3933529	6.5926548
C	4.5748447	3.7611573	4.3187189
C	8.8645083	-2.0062356	4.1909857
H	9.5602806	-2.0478676	3.3547292
C	2.9174743	0.5306718	8.8481422
H	2.0970792	-0.0617566	8.4115356
H	2.4622296	1.2902128	9.5017655
C	3.4051854	2.5007136	7.6483907
H	2.8398623	2.9657373	8.4654946
C	3.8286972	-0.3806316	9.6753388
C	8.3010918	-2.6696350	6.4514464
H	8.5360009	-3.2217994	7.3621477
C	4.2543438	-1.5564816	8.7915352
H	4.7819946	-2.3043965	9.4031266
H	3.3606259	-2.0462314	8.3719327
C	9.1657022	-2.7106411	5.3699289
H	10.0864571	-3.2892868	5.4221164
C	5.0469685	0.3870788	10.2061540
H	5.6618396	0.7920583	9.3898189
H	5.6819955	-0.2688310	10.8171264
H	4.7292069	1.2256650	10.8412419
C	4.4502550	5.1344146	4.4820450
H	4.7053480	5.8245632	3.6798796
C	3.6645684	4.7915740	6.7475266
H	3.3022093	5.1927055	7.6946939
C	3.9907899	5.6471862	5.7076997
H	3.8934813	6.7246878	5.8295837
C	2.9949953	-0.9471905	10.8377857
H	2.6475376	-0.1375714	11.4939332
H	3.5994238	-1.6305552	11.4495057
H	2.1132583	-1.4990478	10.4802623
C	8.1448145	-0.5535140	1.8256505
H	9.1337204	-0.1409012	2.0641987
H	7.6599435	0.0699946	1.0647879
H	8.2273563	-1.5833198	1.4548767
C	5.3281378	3.9875689	2.0058843
H	4.4271870	4.5377764	1.7051926
H	5.6381245	3.3226319	1.1907840
H	6.1469064	4.6764587	2.2502629
Ca	5.2970166	0.7668036	3.3008192

Ni (II)L^{pn} + Ba²⁺

Ni	4.5987757	0.2127613	6.4513838
O	5.5948045	-0.5856199	5.0326637
O	4.2645632	1.5335516	5.1129519
O	7.2141654	-0.6760871	2.9271202
O	4.8569156	3.1459490	3.0837889
N	5.0942586	-1.1726895	7.6368354
N	3.6009143	1.1936492	7.7199245
C	4.2638181	2.8512433	5.3618449
C	6.7806189	-1.1859927	5.2027457
C	7.6785918	-1.2611794	4.1148671
C	7.1525971	-1.7773420	6.4292208
C	6.2123576	-1.8303536	7.5131973
H	6.4518089	-2.5451886	8.3100448
C	3.9326759	3.3745494	6.6301373
C	4.5692605	3.7511456	4.3170642
C	8.9180786	-1.8742556	4.2549322
H	9.6184418	-1.9179951	3.4228476
C	2.8858075	0.5138822	8.8114493
H	2.0649735	-0.0632974	8.3559450
H	2.4295167	1.2747502	9.4632140
C	3.4968398	2.4913294	7.6757256
H	2.9782815	2.9716768	8.5148721
C	3.7700516	-0.4187966	9.6457281
C	8.4078313	-2.4148459	6.5538403
H	8.6798775	-2.8782222	7.5028891
C	4.2163652	-1.5774575	8.7478861

H	4.7385354	-2.3348283	9.3528792
H	3.3321530	-2.0633343	8.3047886
C	9.2841803	-2.4491776	5.4834655
H	10.2571038	-2.9280739	5.5794698
C	4.9781706	0.3329594	10.2204694
H	5.6146635	0.7504811	9.4276694
H	5.5947891	-0.3378852	10.8342821
H	4.6485706	1.1604369	10.8641518
C	4.5758390	5.1237952	4.5374909
H	4.8270999	5.8184800	3.7381608
C	3.9236390	4.7722595	6.8374507
H	3.6548650	5.1653714	7.8186008
C	4.2555633	5.6340397	5.8065286
H	4.2626256	6.7109543	5.9659152
C	2.9066517	-1.0020014	10.7768281
H	2.5453666	-0.2020779	11.4374156
H	3.4941045	-1.6972384	11.3917366
H	2.0322836	-1.5450392	10.3889457
C	8.1047524	-0.7315708	1.7814321
H	9.0372166	-0.1905519	1.9920091
H	7.5791613	-0.2372807	0.9548885
H	8.3137590	-1.7737038	1.5049133
C	5.1912370	4.0350610	1.9847411
H	4.3509893	4.7062459	1.7621198
H	5.3815480	3.3947062	1.1141672
H	6.0976707	4.6102254	2.2166775
Ba	4.7394695	0.4388822	2.9077830

Ni (II)L^{Pn} + Li⁺+ClO₄⁻¹

Ni	4.8607741	0.2404598	6.3615026
O	6.1480794	-0.1897823	5.0930532
O	4.5030391	1.5151655	5.0095570
O	7.5306685	-0.4093902	2.9273564
O	5.0460022	3.1619046	3.0588289
N	5.3539766	-1.1955296	7.4883355
N	3.6099075	1.0565241	7.5247008
C	4.2110377	2.7727126	5.2114095
C	7.1134072	-1.0660757	5.1327615
C	7.9222818	-1.2092558	3.9656535
C	7.3690756	-1.8936158	6.2508357
C	6.4412990	-1.9162048	7.3252766
H	6.6303601	-2.6825410	8.0885330
C	3.6228440	3.2495356	6.4117258
C	4.4783298	3.7179580	4.1693486
C	8.9763459	-2.1062114	3.9595444
H	9.5833092	-2.2299356	3.0642865
C	2.9474557	0.3055591	8.5944114
H	2.2056182	-0.3644072	8.1279186
H	2.3954520	1.0085842	9.2405344
C	3.2742375	2.3196385	7.4347206
H	2.6226424	2.7100865	8.2281390
C	3.9053638	-0.5292180	9.4507636
C	8.4649287	-2.8007540	6.2245513
H	8.6504142	-3.4368028	7.0918686
C	4.4774840	-1.6489308	8.5762283
H	5.0363115	-2.3536104	9.2146965
H	3.6425754	-2.2110357	8.1239645
C	9.2563686	-2.8944058	5.1011774
H	10.0895942	-3.5958241	5.0700674
C	5.0242130	0.3418604	10.0355441
H	5.6230256	0.8032434	9.2388582
H	5.6963567	-0.2616613	10.6624098
H	4.6061924	1.1449524	10.6605089
C	4.1797925	5.0619579	4.3460615
H	4.4040463	5.7783810	3.5568177
C	3.3084946	4.6262423	6.5607445
H	2.8469785	4.9674186	7.4891078
C	3.5902615	5.5179588	5.5469899
H	3.3612274	6.5770368	5.6607181
C	3.0855726	-1.1811404	10.5752324
H	2.6324805	-0.4146596	11.2205187
H	3.7251494	-1.8143089	11.2067624
H	2.2759638	-1.8097907	10.1742144
C	8.0817387	-0.6996183	1.6333485
H	9.1726459	-0.5433386	1.6261865
H	7.6039956	0.0057410	0.9474544
H	7.8294815	-1.7292828	1.3412218

C	5.4647582	4.0319761	2.0053727
H	4.6071191	4.5652391	1.5619780
H	5.9231396	3.3770158	1.2570684
H	6.2040365	4.7656041	2.3673622
Li	5.3742047	0.5051415	3.3432572
O	5.2745386	0.8755860	1.3274912
H	5.1792158	-0.0880539	1.0648251
H	4.4026233	1.2619277	1.1429874
Cl	4.5904744	-2.2968702	2.3348559
O	5.0836542	-1.7745997	1.0205277
O	5.6892892	-2.9712196	3.0181758
O	3.4663055	-3.1857804	2.1189386
O	4.1494406	-1.1228560	3.1436092

Ni (II)Lⁿ + Ba²⁺ +2ClO₄⁻¹

Ba	15.9468685	5.8108634	10.3373801
Ni	12.7156211	5.8005194	12.0477406
Cl	18.8760245	4.2543826	9.6133546
O	14.4983844	6.0839600	12.5492397
O	17.0697115	5.9723121	12.9896054
O	14.9000080	3.7196174	8.7159561
O	13.4664239	4.6729015	10.7238582
N	10.9832627	5.1685729	11.7946369
N	12.1158285	7.2589775	13.0344017
C	14.9372937	6.7819150	13.5785341
C	14.1200143	7.6277116	14.3705684
O	20.0798675	4.6040173	10.3432464
O	17.8240555	3.7869404	10.5762837
C	11.3987524	3.8356498	9.7883043
C	13.5441848	3.4702781	8.6882178
C	12.8084017	4.0308427	9.7805649
C	10.5975059	4.3569276	10.8488309
H	9.5503334	4.0263266	10.8756607
C	16.3323262	6.7263965	13.8751047
C	18.4800673	5.8180778	13.2480118
H	18.8573844	5.1591495	12.4602699
H	18.6401461	5.3530435	14.2324773
H	18.9914738	6.7914054	13.2000709
C	12.9029324	2.7503538	7.6907513
H	13.4770968	2.3368825	6.8636441
O	18.3073747	5.4745340	8.9519449
C	12.7836994	7.9023826	13.9471209
H	12.3069078	8.7936300	14.3745623
C	10.8903902	7.8582124	12.4982732
H	11.0448442	7.9544532	11.4145123
H	10.7693692	8.8786401	12.8936416
O	19.1141871	3.2290951	8.6156873
C	16.8497233	7.4075040	14.9670169
H	17.9124228	7.3472322	15.1943279
C	14.6754423	8.3351727	15.4663132
H	14.0309751	8.9922037	16.0525724
C	10.0202039	5.5257659	12.8404247
H	10.4895064	5.2938615	13.8071131
H	9.1146183	4.9048428	12.7497989
C	11.5082030	2.5498735	7.7288738
H	11.0265733	1.9785160	6.9364688
C	16.0139132	8.2070468	15.7742026
H	16.4426562	8.7440074	16.6194069
C	15.7246497	3.0449078	7.7416545
H	15.4940906	3.4000356	6.7257038
H	15.5794945	1.9568655	7.8072570
H	16.7612879	3.2863702	7.9936412
C	10.7694330	3.0827651	8.7632957
H	9.6882826	2.9397962	8.8037750
C	9.6294795	7.0185338	12.8015510
C	8.5954974	7.2707979	11.6963240
H	8.3918637	8.3463174	11.5893098
H	7.6436198	6.7694605	11.9260849
H	8.9580718	6.9016842	10.7255564
C	9.0603456	7.3946313	14.1770663
H	9.8316707	7.3159573	14.9581499
H	8.2279886	6.7317445	14.4571938
H	8.6806811	8.4262869	14.1710779
Cl	14.5007203	8.8806906	10.3258623
O	13.9512700	7.6397569	9.6851297
O	14.6727903	9.9165827	9.3315292
O	15.8295525	8.4896130	10.8969520

o 13.6137278 9.3043028 11.4002072