

Supplementary information

Synthesis, spectroscopic, biological activities and DFT calculations of nickel(II) mixed-ligand complexes of tridentate Schiff bases

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¹³C-NMR DATA

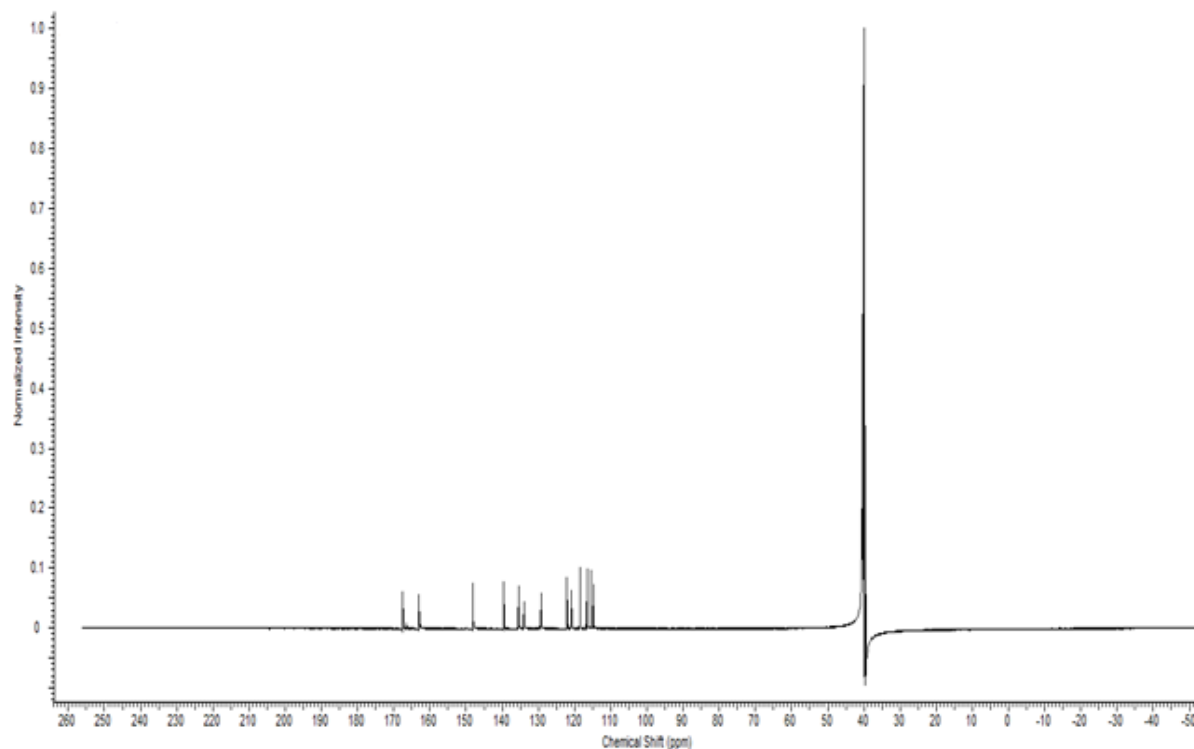


Figure S1. ¹³C NMR of NiL₁NH₃ complex.

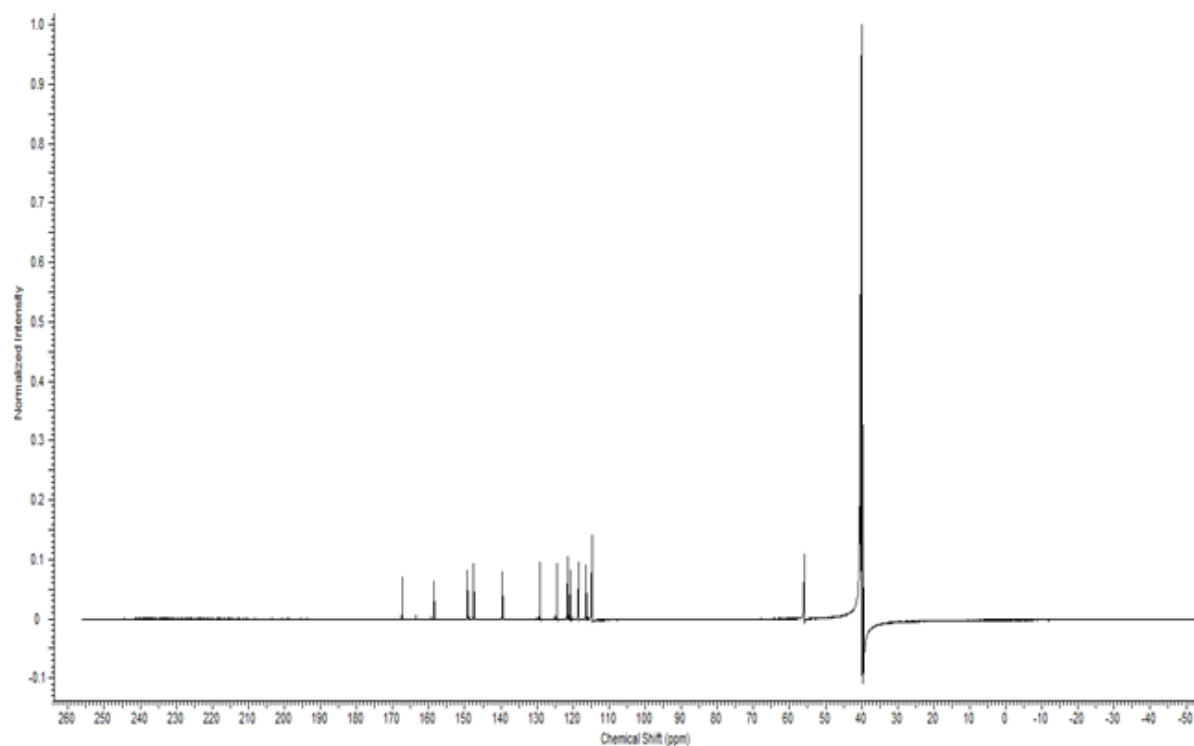


Figure S2. ^{13}C NMR of NiL_2NH_3 complex.

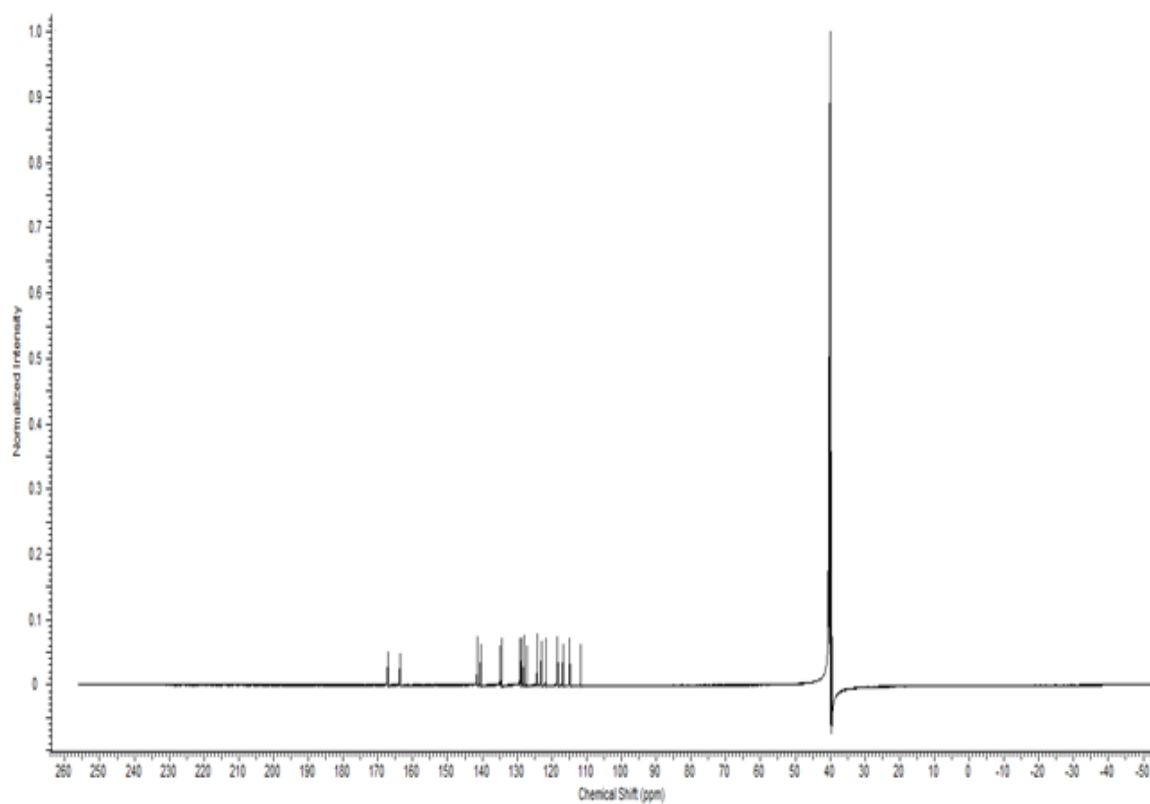


Figure S3. ^{13}C NMR of NiL_3NH_3 .

Table S1. Selected bond distances and bond angles.

NiL ₁ NH ₃			NiL ₂ NH ₃			NiL ₃ NH ₃		
Bond (Å)	B3LYP	EDF1	Bond (Å)	B3LYP	EDF1	Bond (Å)	B3LYP	EDF1
Ni1–N1	1.844	1.818	Ni1–N1	1.845	1.817	Ni1–N1	1.834	1.811
Ni1–N2	1.936	1.944	Ni1–N2	1.938	1.940	Ni1–N2	1.939	1.943
Ni1–O1	1.818	1.807	Ni1–O1	1.814	1.807	Ni1–O1	1.813	1.801
Ni1–O2	1.825	1.825	Ni1–O2	1.827	1.825	Ni1–O2	1.823	1.823
O2–C9	1.327	1.332	O2–C9	1.327	1.331	O2–C15	1.328	1.333
O1–C4	1.310	1.317	O1–C4	1.314	1.322	O1–C8	1.306	1.315
N1–C7	1.307	1.322	N1–C7	1.307	1.322	N1–C11	1.312	1.326
N1–C8	1.418	1.418	N1–C8	1.417	1.417	N1–C12	1.418	1.417
C3–C4	1.432	1.338	C3–C4	1.432	1.437	C12–C15	1.416	1.419
C3–C7	1.427	1.423	C3–C7	1.428	1.425	C7–C11	1.424	1.424
C8–C9	1.415	1.418	C8–C9	1.416	1.419	C7–C8	1.424	1.430
Bond angles (o)								
N1–Ni1–N2	176.19	174.63	N1–Ni1–N2	174.83	175.69	N1–Ni1–N2	176.37	175.97
O1–Ni1–O2	174.78	173.60	O1–Ni1–O2	174.62	173.34	O1–Ni1–O2	175.35	174.06
N1–Ni1–O2	88.21	88.40	N1–Ni1–O2	88.04	88.51	N2–Ni1–O2	87.85	87.22
N1–Ni1–O1	97.00	94.60	N1–Ni1–O1	97.33	98.15	N2–Ni1–O1	87.60	87.02
N2–Ni1–O2	87.98	86.23	N2–Ni1–O2	86.80	87.18	N1–Ni1–O1	96.02	96.98
N2–Ni1–O1	86.81	87.37	N2–Ni1–O1	87.83	86.16	N1–Ni1–O2	88.52	88.79
Ni1–N1–C8	111.00	111.76	Ni1–N1–C8	111.12	111.73	Ni1–O2–C15	111.44	111.26
Ni1–N1–C7	125.23	124.98	Ni1–N1–C7	125.21	125.05	Ni1–O1–C8	127.74	127.39
Ni1–O2–C9	111.66	111.69	Ni1–O2–C9	111.81	111.44	Ni1–N1–C11	125.61	125.30
Ni1–O1–C4	127.14	126.68	Ni1–O1–C4	126.63	126.40	Ni1–N1–C12	111.00	111.64
N1–C8–C9	111.24	111.00	N1–C8–C9	111.28	110.99	N1–C12–C15	111.28	111.03
N1–C7–C3	125.10	125.14	N1–C7–C3	124.97	125.06	N1–C11–C7	125.84	125.89
O1–C4–C3	123.56	123.52	O1–C4–C3	123.96	123.67	O2–C15–C12	117.75	117.25
O2–C9–C8	117.88	117.23	O2–C9–C8	117.74	117.34	O1–C8–C7	124.46	124.21
C4–C3–C7	121.96	121.68	C4–C3–C7	121.89	121.67	C8–C7–C11	120.28	120.10