Electronic Supplementary Material (ESI) for RSC Advances.

Physicochemical Investigations of the Metal Complexes of L-Valine with Doubly Charged Ions of Nickel, Copper and Zinc: A Combined Experimental and Computational Approach

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Table S1 Calculated ZPVE values, total electronic energies[a], Gibbs free energies as well as ZPVE corrected values (scaled with 0.9877) of total electronic energies (E_{corr}) and Gibbs free energies (G_{corr}) of the representative reaction species in gas and aqueous phase.

Systems	Phases	ZPVE	Total Energy (E)	Gibbs Energy (G)	E_{corr}	G_{corr}
L-Val	Aqueous	0.165205	-402.5128732	-402.381866	-402.349700	-402.2186930
	Gas	0.164482	-402.5006506	-402.370308	-402.3381917	-402.2078491
$Ni(L\text{-}Val)_2$	Aqueous	0.311212	-2312.2337146	-2311.971268	-2311.926331	-2311.663884
	Gas	0.311197	-2312.1989958	-2311.936258	-2311.891627	-2311.628889
$Cu(L\text{-}Val)_2$	Aqueous	0.309547	-2444.3998593	-2444.140873	-2444.094120	-2443.835133
	Gas	0.309158	-2444.3625356	-2444.104078	-2444.057180	-2443.798723
$Zn(L\text{-}Val)_2$	Aqueous	0.308920	-2583.2811777	-2583.022465	-2582.976057	-2582.717345
	Gas	0.308736	-2583.229164	-2582.971494	-2582.924225	-2582.666555

[a]energies in Hartrees

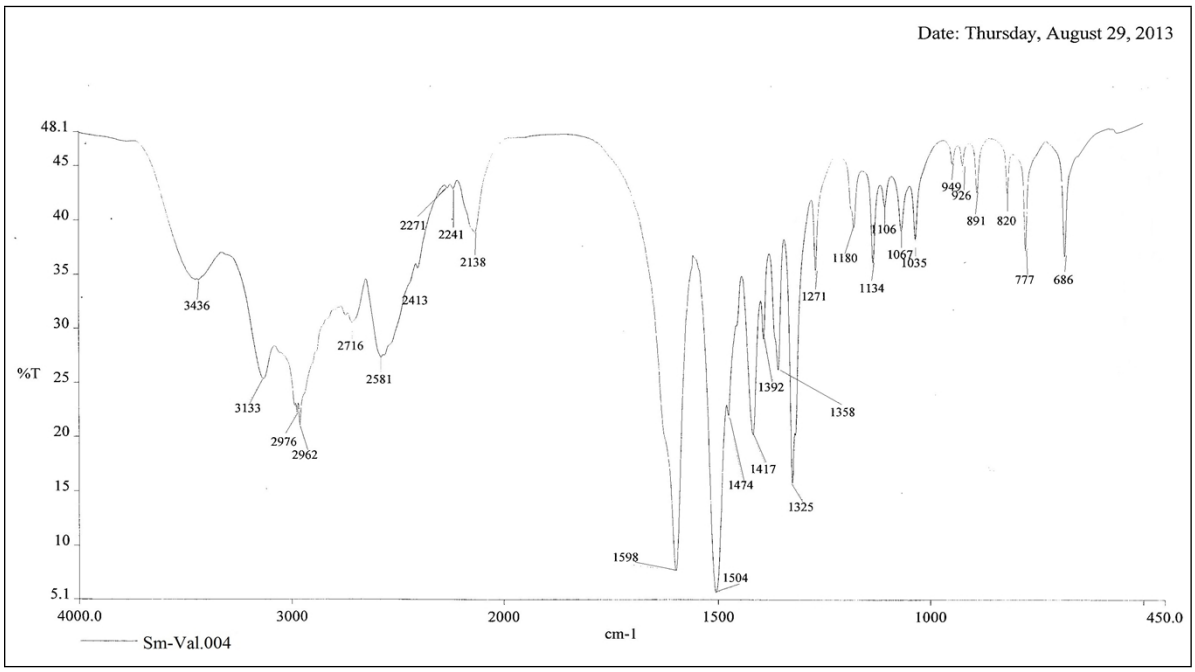
Table S2 Mulliken, NPA and ESP charges for some of the chemically meaningful atoms in the three metal complex calculated at B3LYP/6-311++G(d,p) level. Gas phase values are given in parentheses.

Atoms	L-Val			$Ni(L\text{-}Val)_2$		
	Mulliken	NPA	ESP	Mulliken	NPA	ESP
M[a]	-------	---------	--------	-0.003693 (-0.032036)	1.03491 (0.99067)	0.502207 (0.363593)
N_6	-0.073736 (-0.447348)	-0.70089 (-0.87261)	-0.524801 (-0.968575)	-0.104232 (-0.145984)	-0.80757 (-0.79516)	-0.318920 (-0.311839)
O_7	-0.490174 (-0.173492)	-0.80589 (-0.68617)	-0.806145 (-0.548369)	-0.460296 (-0.359505)	-0.78615 (-0.77554)	-0.731582 (-0.661102)
C_1	0.042854 (-0.134683)	0.76753 (0.79590)	0.814707 (0.628347)	0.196400 (0.103068)	0.79883 (0.77959)	0.878067 (0.809040)
C_2	-0.614625 (-0.147382)	-0.10222 (-0.12097)	0.035038 (0.192809)	-0.416980 (-0.380376)	-0.12045 (-0.11559)	-0.194097 (-0.213722)
O_8	-0.463348 (-0.285490)	-0.76271 (-0.59080)	-0.801261 (-0.520484)	-0.439964 (-0.304248)	-0.70689 (-0.62040)	-0.722445 (-0.601708)
H_a (NH_2)	0.315189 (0.265827)	0.43101 (0.36375)	0.342829 (0.362506)	0.361725 (0.312369)	0.41263 (0.38666)	0.274185 (0.261088)
H_b (NH_2)	0.346459 (0.270288)	0.43910 (0.37300)	0.381177 (0.376448)	0.383811 (0.356346)	0.41818 (0.40036)	0.298942 (0.285161)
C_3	0.394880 (0.194510)	-0.23722 (-0.23429)	0.405580 (0.335989)	0.304013 (0.311129)	-0.23740 (-0.23791)	0.513277 (0.454087)
C_4	-0.503593 (-0.580755)	-0.57796 (-0.57631)	-0.472765 (-0.421232)	-0.665815 (-0.617934)	-0.58208 (-0.57970)	-0.436589 (-0.405834)
C_5	-0.675291 (-0.574236)	-0.57070 (-0.57786)	-0.606361 (-0.529934)	-0.629292 (-0.612809)	-0.57641 (-0.57760)	-0.553507 (-0.552061)

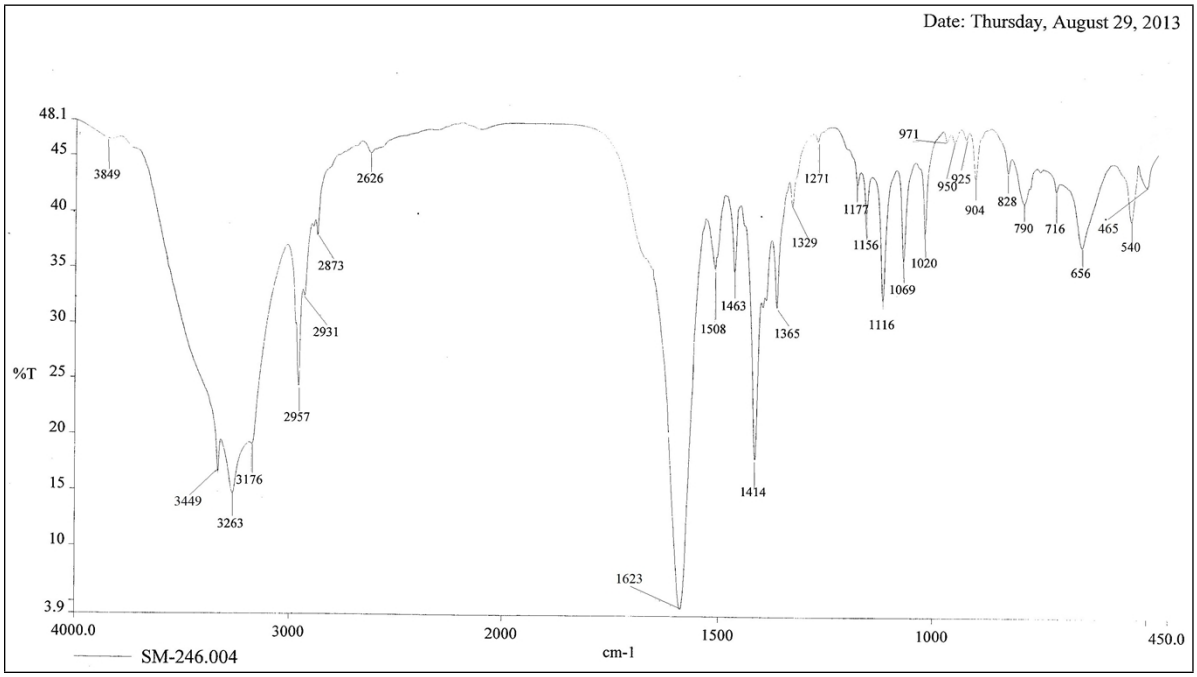
[a]M=Ni(II), Cu(II) or Zn(II); Atomic charges in a. u

Table S2 Continued…….

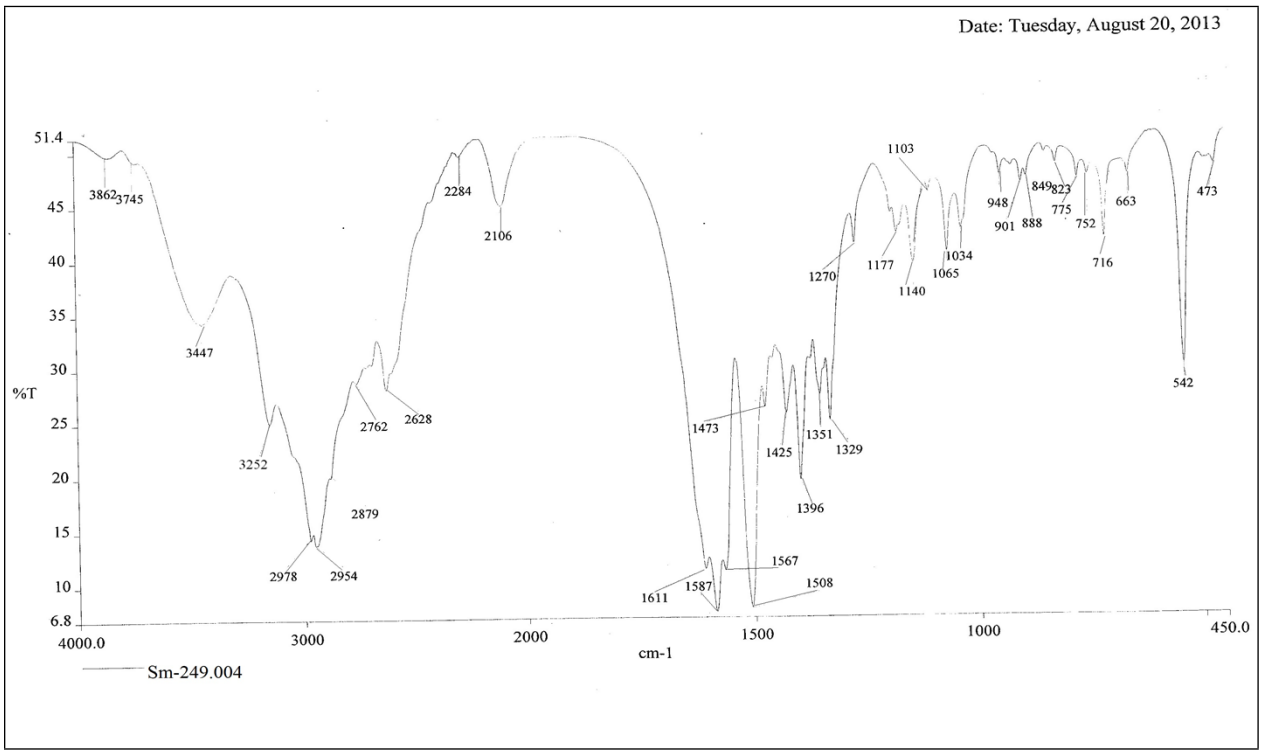
Atom No.	$Cu(L\text{-}Val)_2$			$Zn(L\text{-}Val)_2$		
	Mulliken	NPA	ESP	Mulliken	NPA	ESP
M	-0.131079 (-0.173597)	1.32012 (1.28338)	0.752720 (0.621541)	0.202870 (0.158905)	1.62942 (1.62149)	1.330027 (1.198714)
N_6	0.014881 (-0.042217)	-0.87429 (-0.86423)	-0.388360 (-0.370625)	0.019776 (-0.029815)	-0.96342 (-0.95326)	-0.991929 (-1.107260)
O_7	-0.398997 (-0.294665)	-0.84383 (-0.83647)	-0.798074 (-0.723608)	-0.334723 (-0.228336)	-0.90051 -0.90294)	-0.789079 (-0.739991)
C_1	0.202292 (0.108631)	0.80134 (0.78028)	0.905859 (0.836163)	0.189042 (0.087134)	0.79680 (0.77819)	0.780150 (0.777671)
C_2	-0.527983 (-0.487464)	-0.12098 (-0.11471)	-0.202976 (-0.232321)	-0.646553 (-0.572509)	-0.12675 (-0.11839)	0.081099 (-0.064887)
O_8	-0.446266 (-0.304409)	-0.71638 (-0.62633)	-0.735247 (-0.608931)	-0.454727 (-0.297893)	-0.73433 (-0.63756)	-0.748616 (-0.613300)
H_a (NH_2)	0.348705 (0.299312)	0.41265 (0.38576)	0.273266 (0.253406)	0.288940 (0.249390)	0.40880 (0.39109)	0.377581 (0.412972)
H_b (NH_2)	0.371367 (0.343399)	0.41672 (0.39785)	0.296302 (0.281381)	0.366626 (0.315961)	0.42375 (0.38651)	0.426338 (0.436419)
C_3	0.353259 (0.367420)	-0.23843 (-0.23921)	0.569771 (0.487411)	0.224141 (0.207000)	-0.23796 (-0.24650)	0.515575 (0.580695)
C_4	-0.685223 (-0.639426)	-0.58312 (-0.57964)	-0.450012 (-0.411816)	-0.637857 (-0.626475)	-0.57973 (-0.57727)	-0.473256 (-0.430441)
C_5	-0.626760 (-0.607293)	-0.57725 (-0.57537)	-0.621980 (-0.558750)	-0.586382 (-0.552731)	-0.58853 (-0.58449)	-0.377984 (-0.314581)



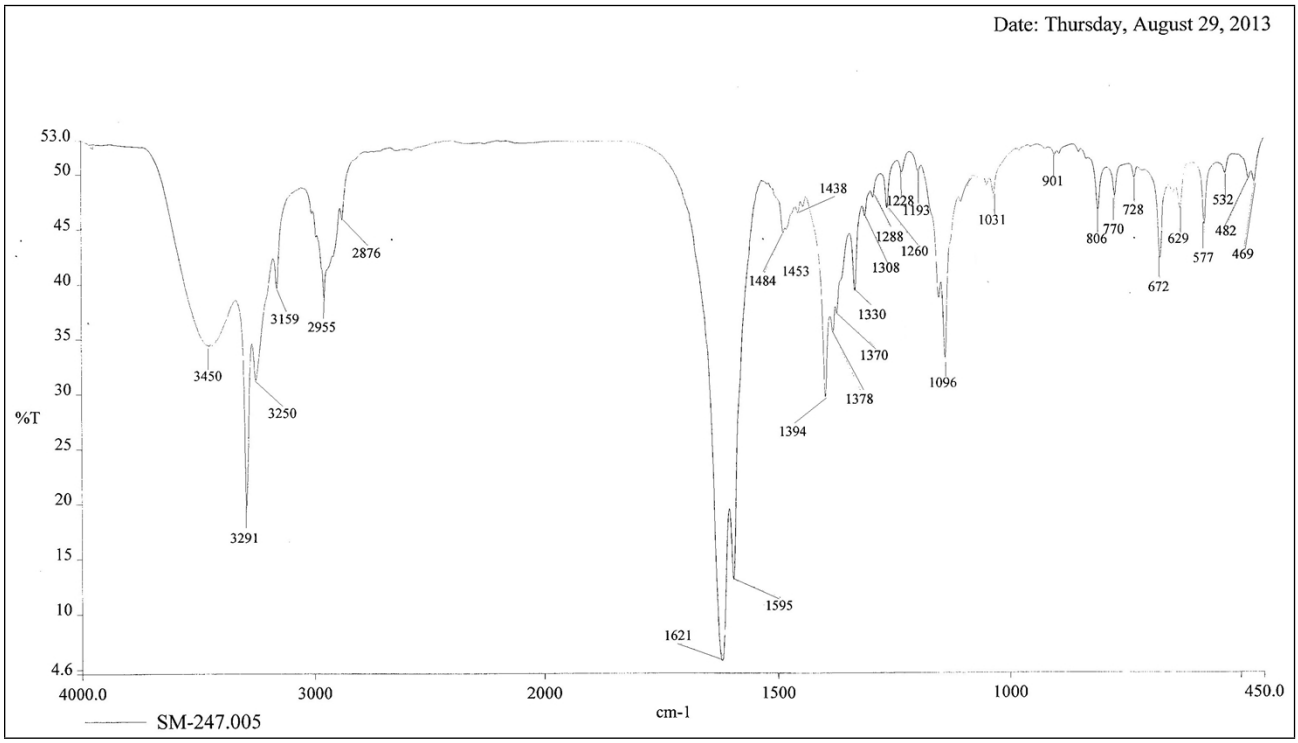
Experimental FT-IR spectra for L-Val in Solid state



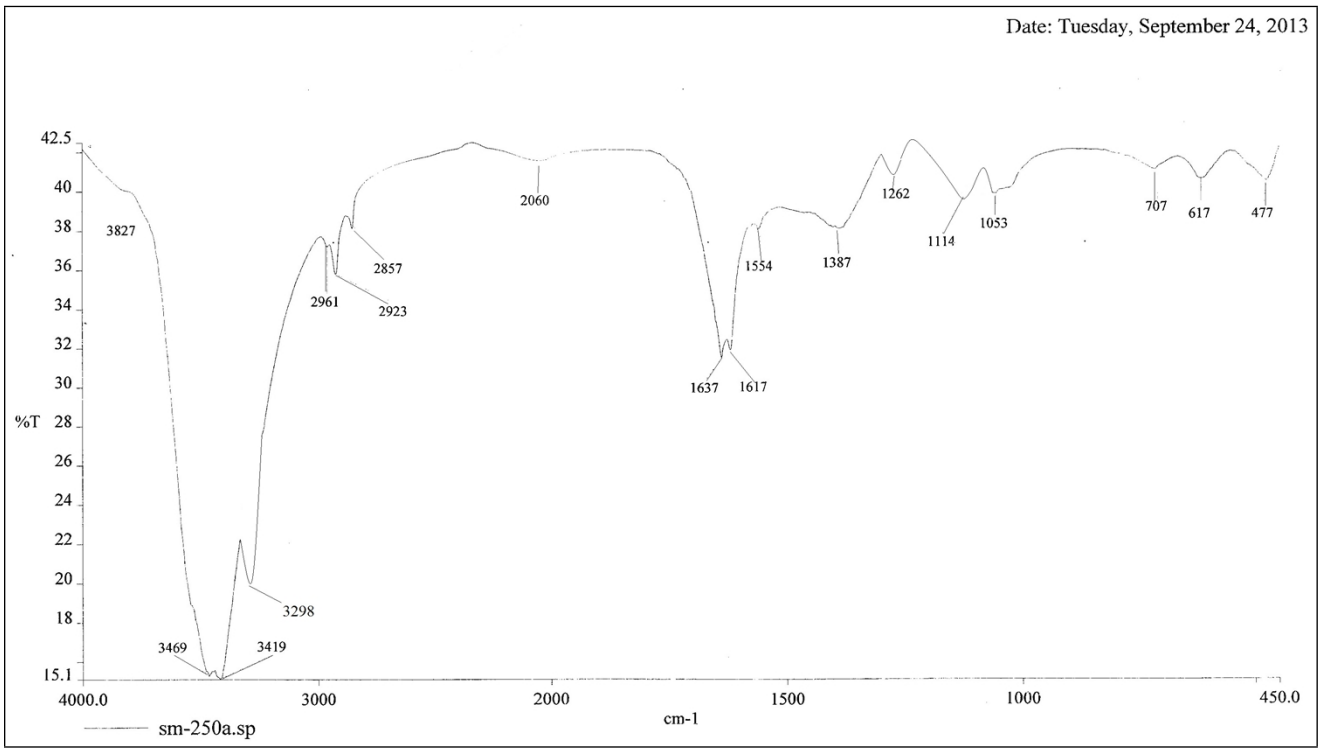
Experimental FT-IR spectra for $Ni(L\text{-}Val)_2$ complex (solid state technique)



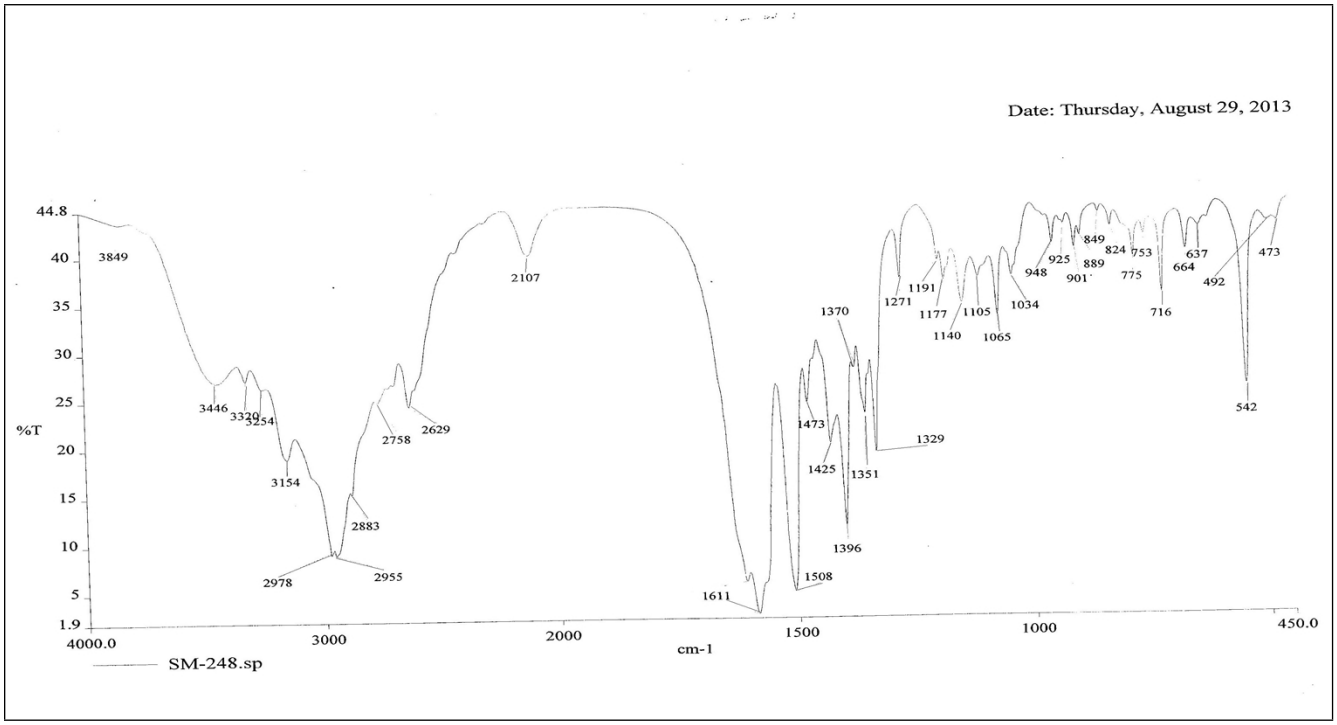
Experimental FT-IR spectra for Ni(L-Val)$_2$ complex (Co-precipitation technique)



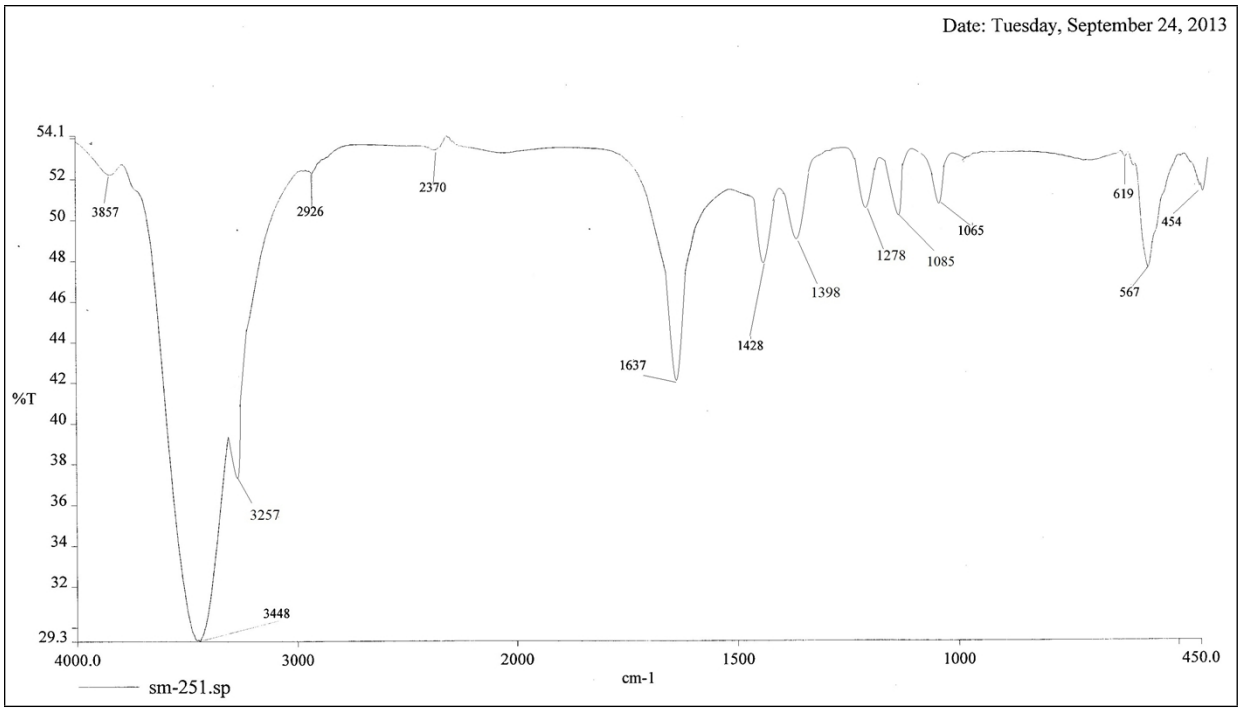
Experimental IR spectra for Cu(L-Val)$_2$ complex (solid state technique)



Experimental FT-IR spectra for $Cu(L\text{-}Val)_2$ complex (Co-precipitation technique)

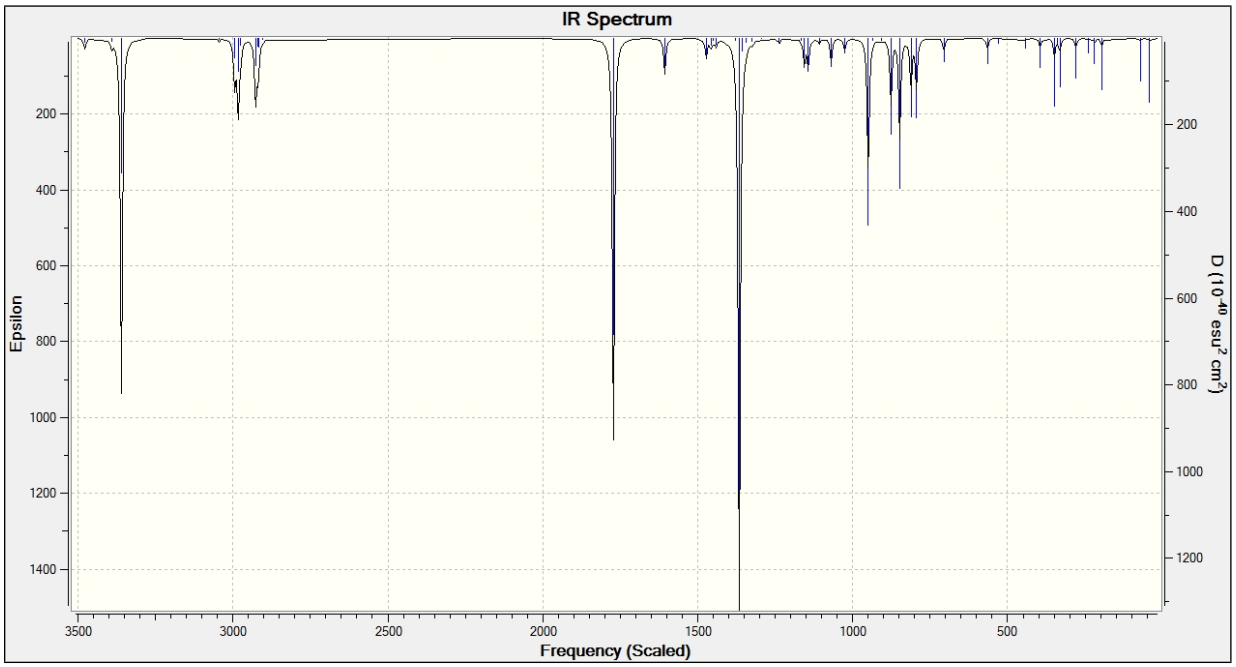


Experimental FT-IR spectra for $Zn(L\text{-}Val)_2$ complex (solid state technique)

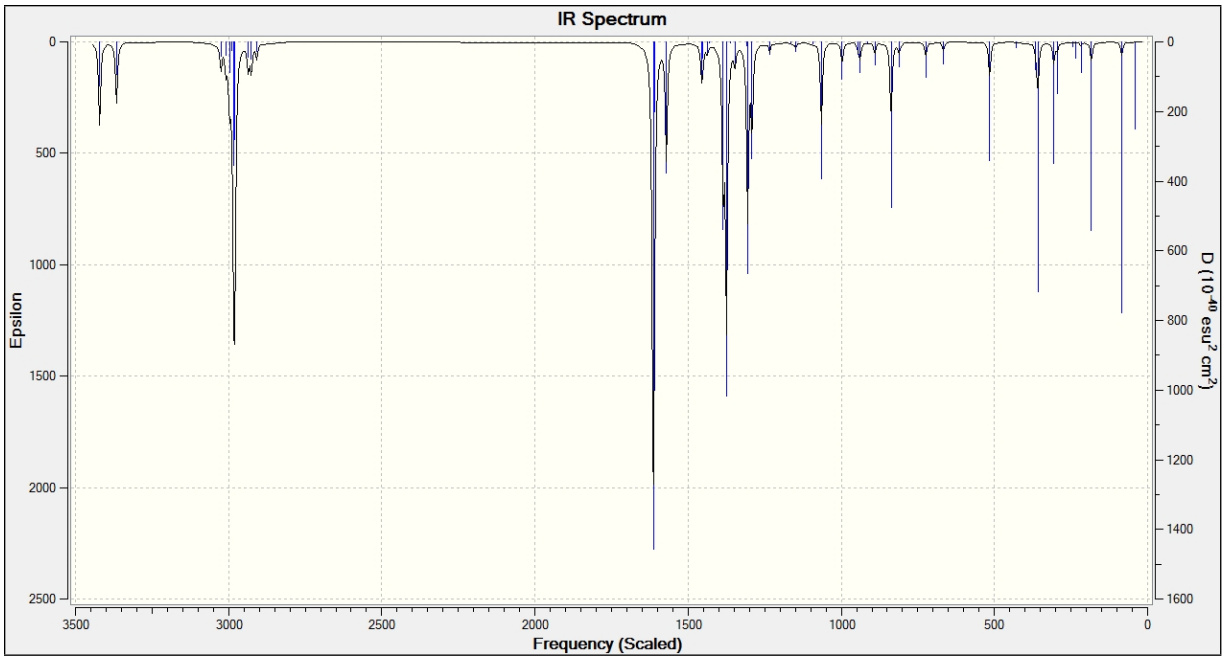


Experimental FT-IR spectra for $Zn(L\text{-}Val)_2$ complex (Co-precipitation technique)

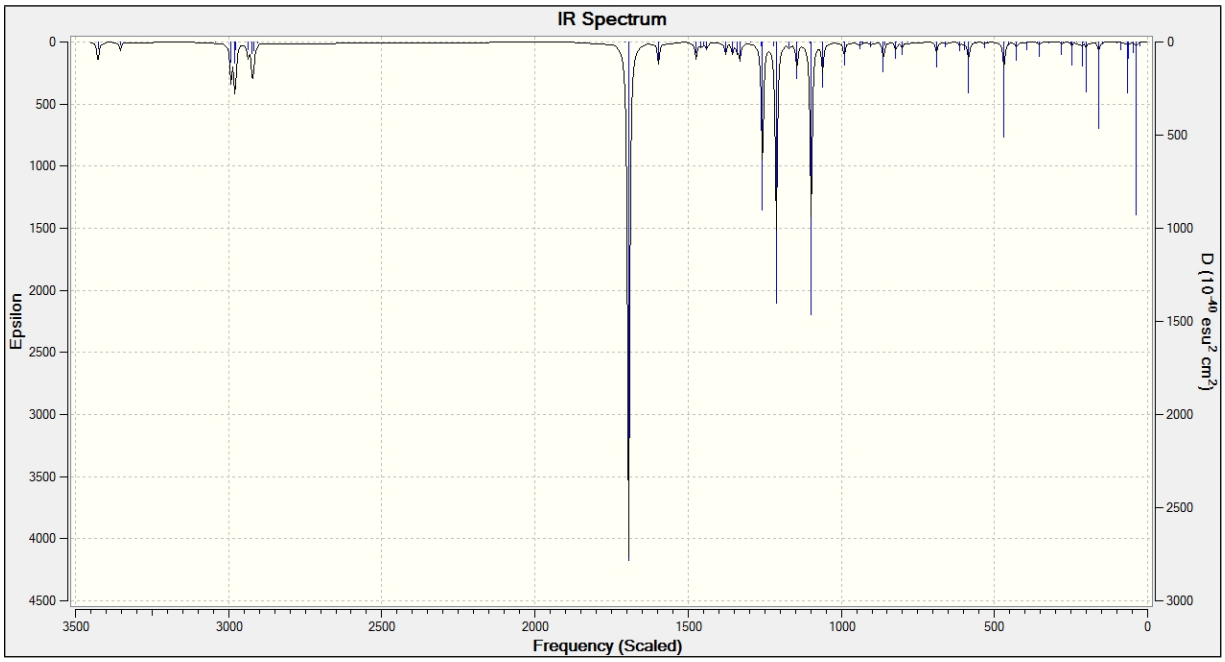
Fig. S1 Experimental FT-IR spectra for L-Val and its metal complexes



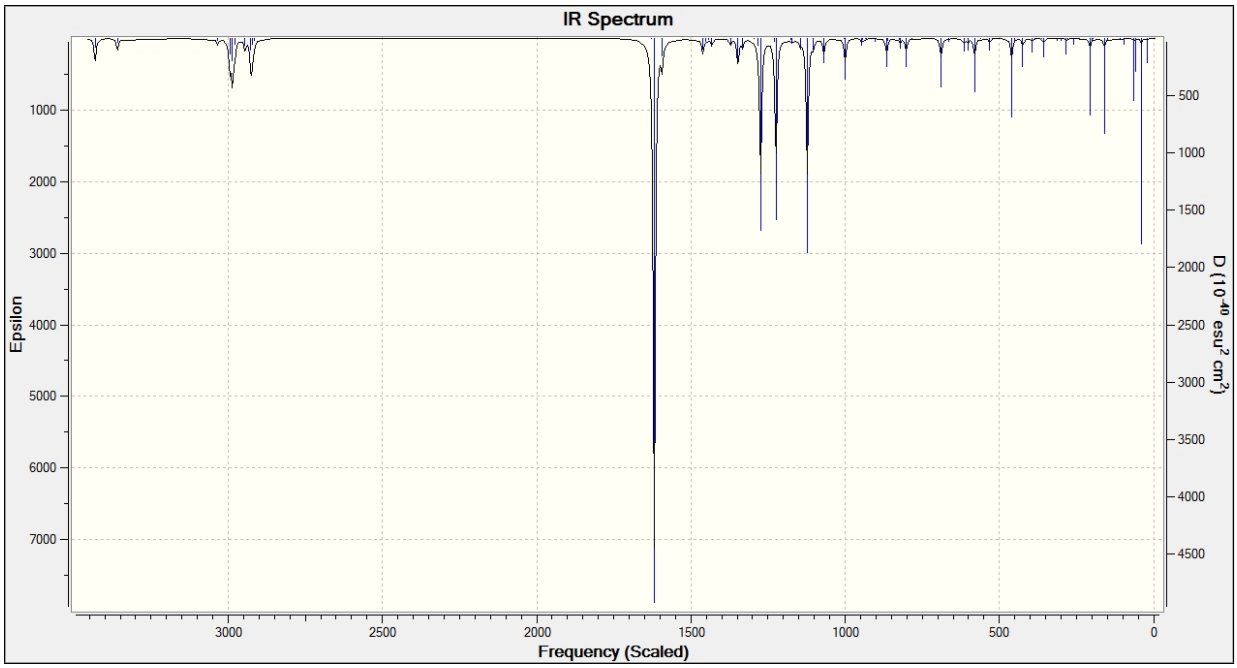
Theoretical IR spectra for L-Val in gas phase



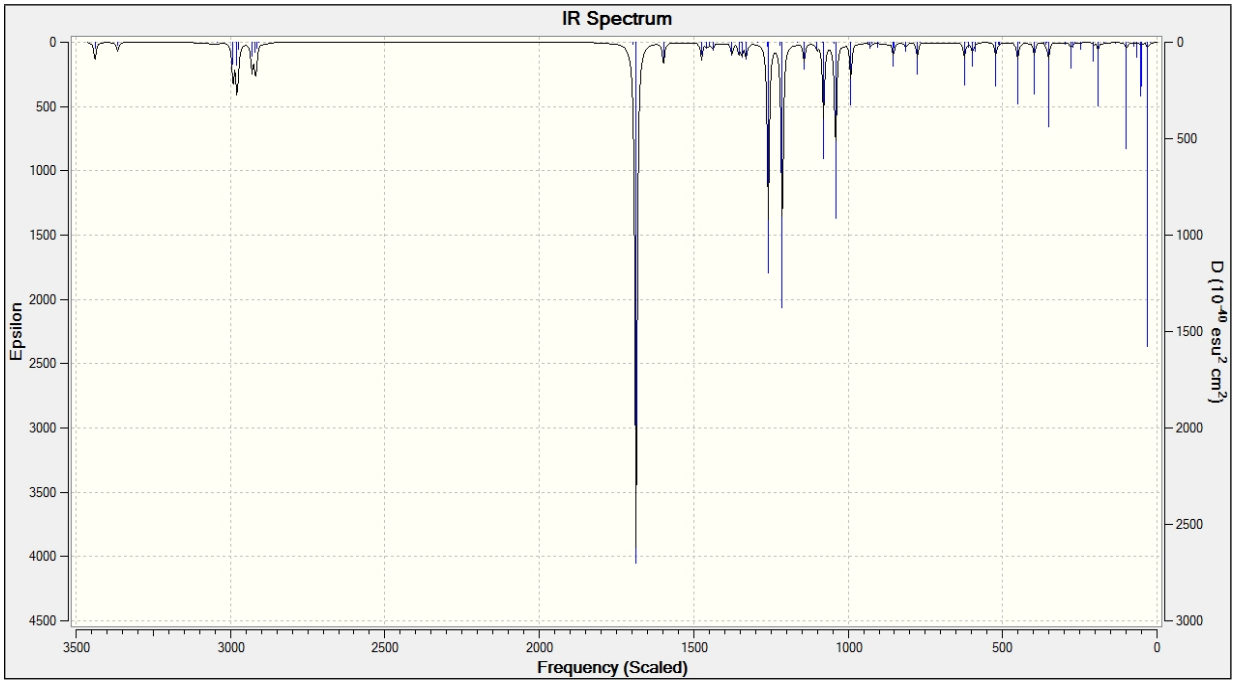
Theoretical IR spectra for L-Val in aqueous phase



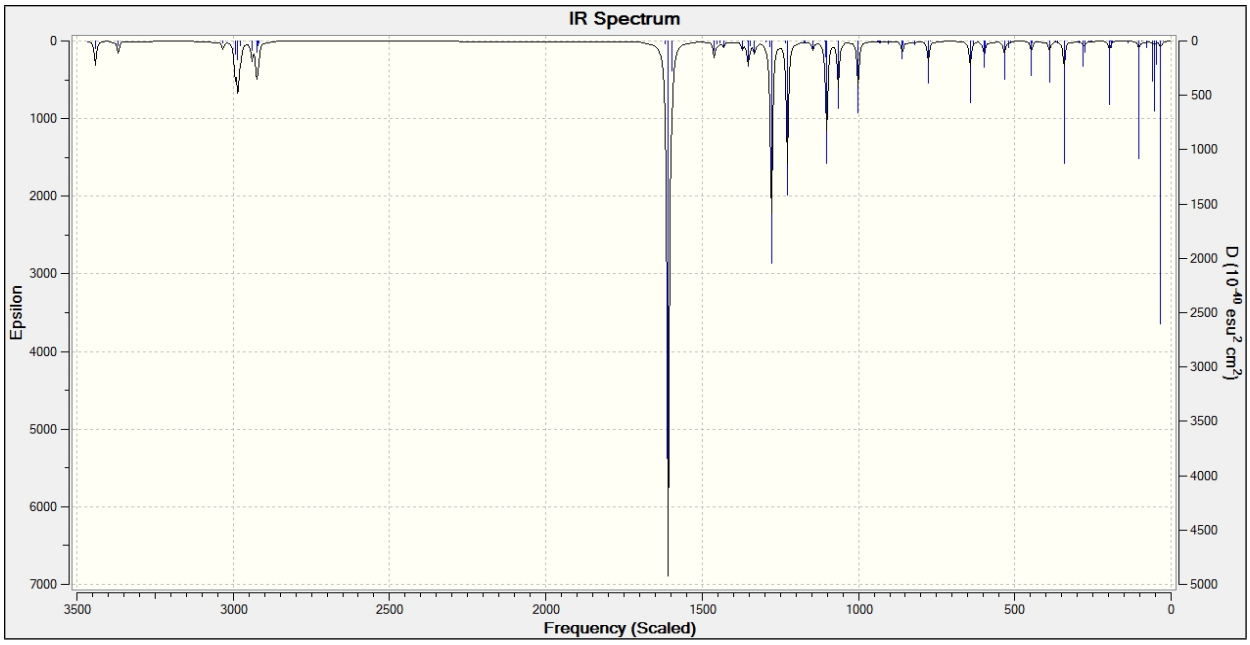
Theoretical IR spectra for $Ni(L\text{-}Val)_2$ in gas phase



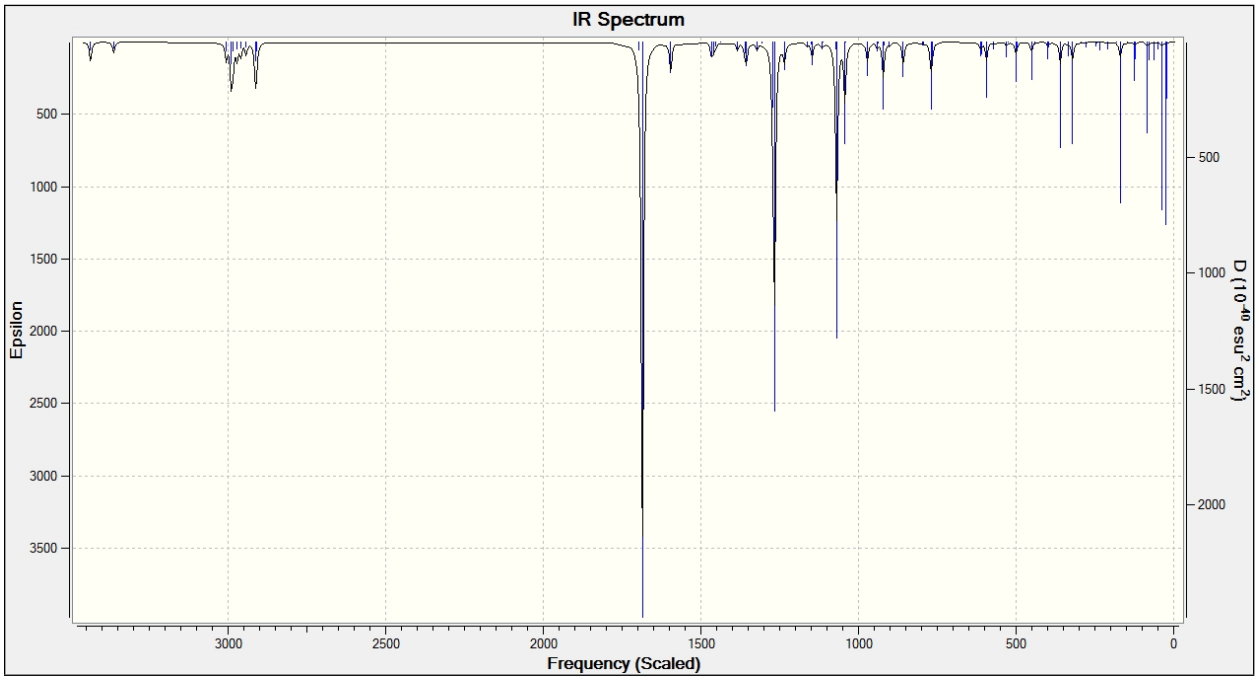
Theoretical IR spectra for $Ni(L\text{-}Val)_2$ in aqueous phase



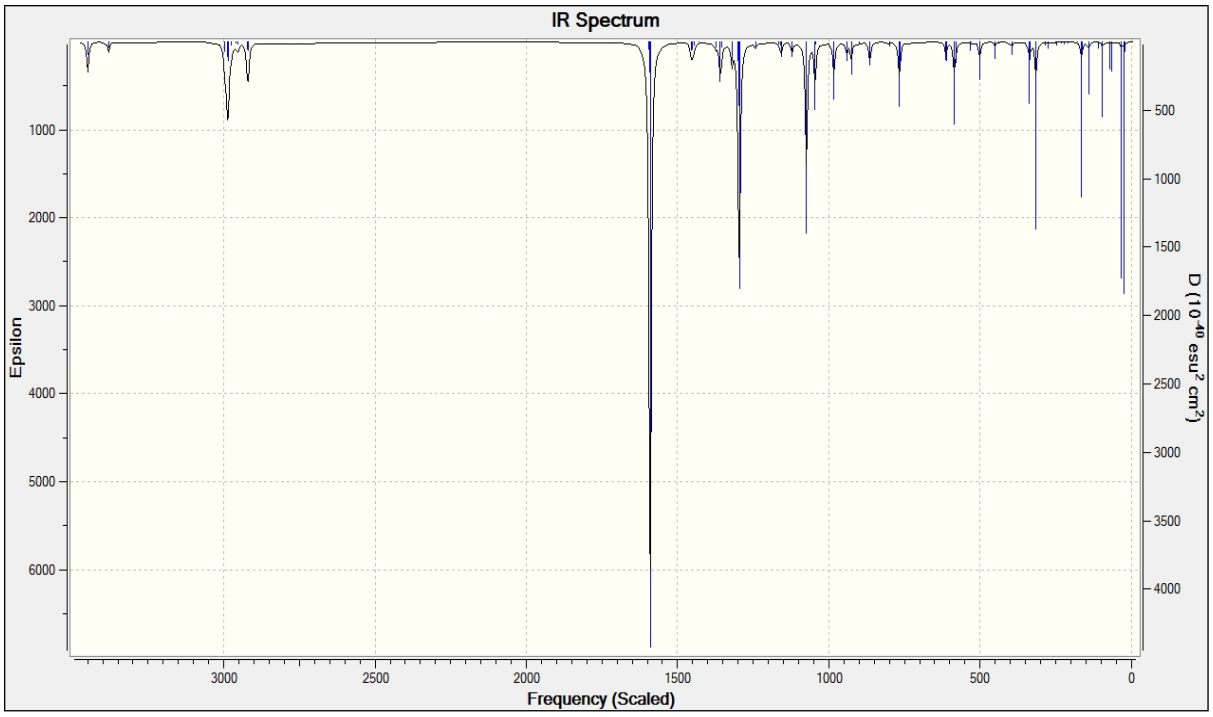
Theoretical IR spectra for $Cu(L\text{-}Val)_2$ in gas phase



Theoretical IR spectra for $Cu(L\text{-}Val)_2$ in aqueous phase

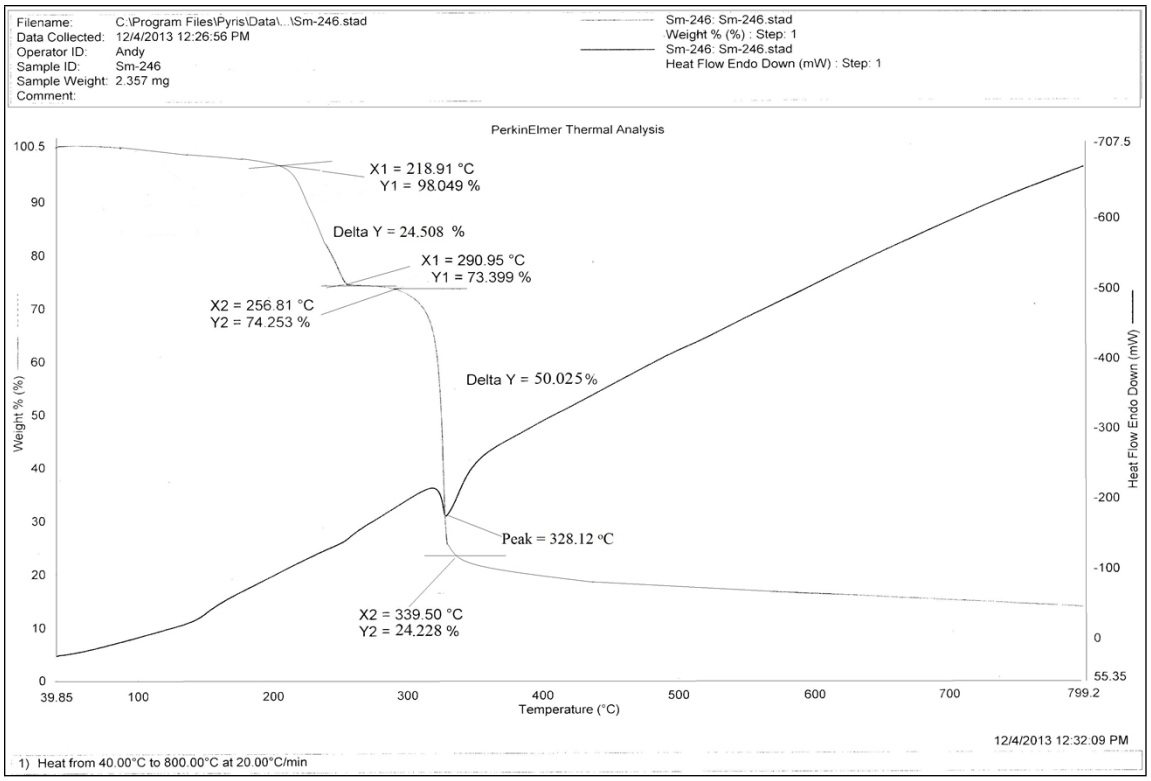


Theoretical IR spectra for $Zn(L\text{-}Val)_2$ in gas phase

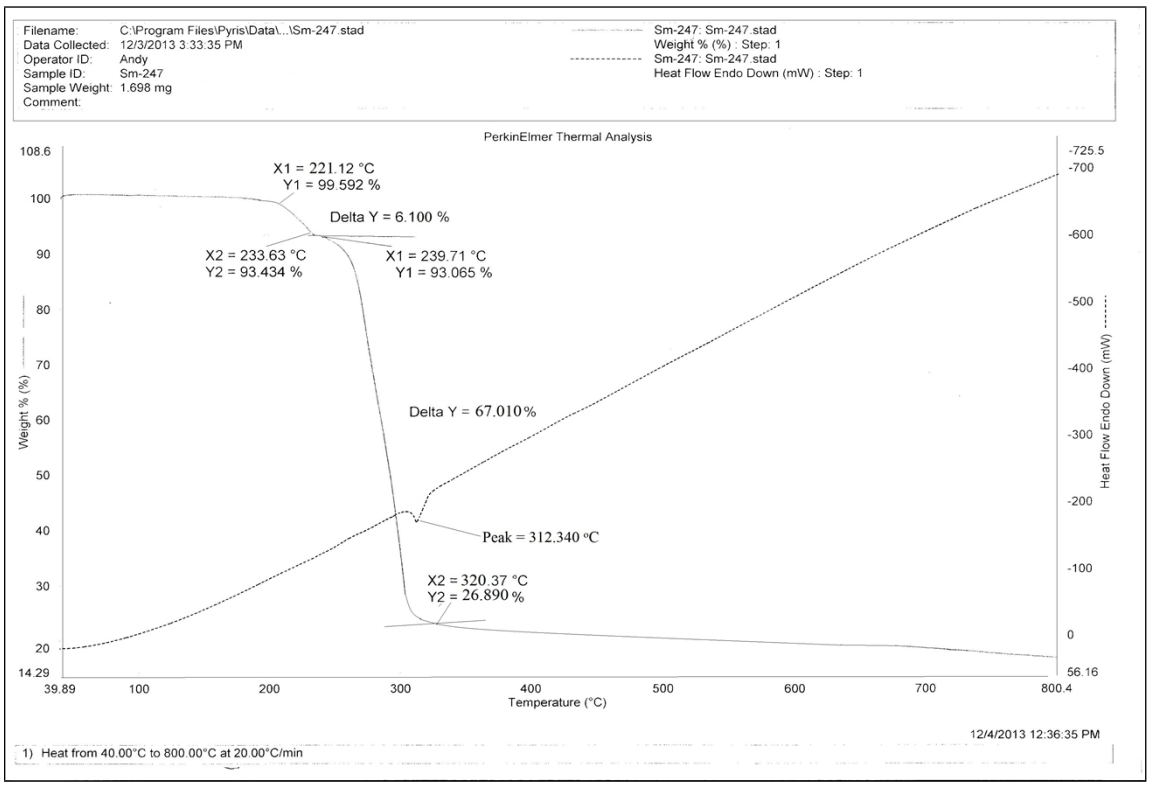


Theoretical IR spectra for $Zn(L\text{-}Val)_2$ in aqueous phase

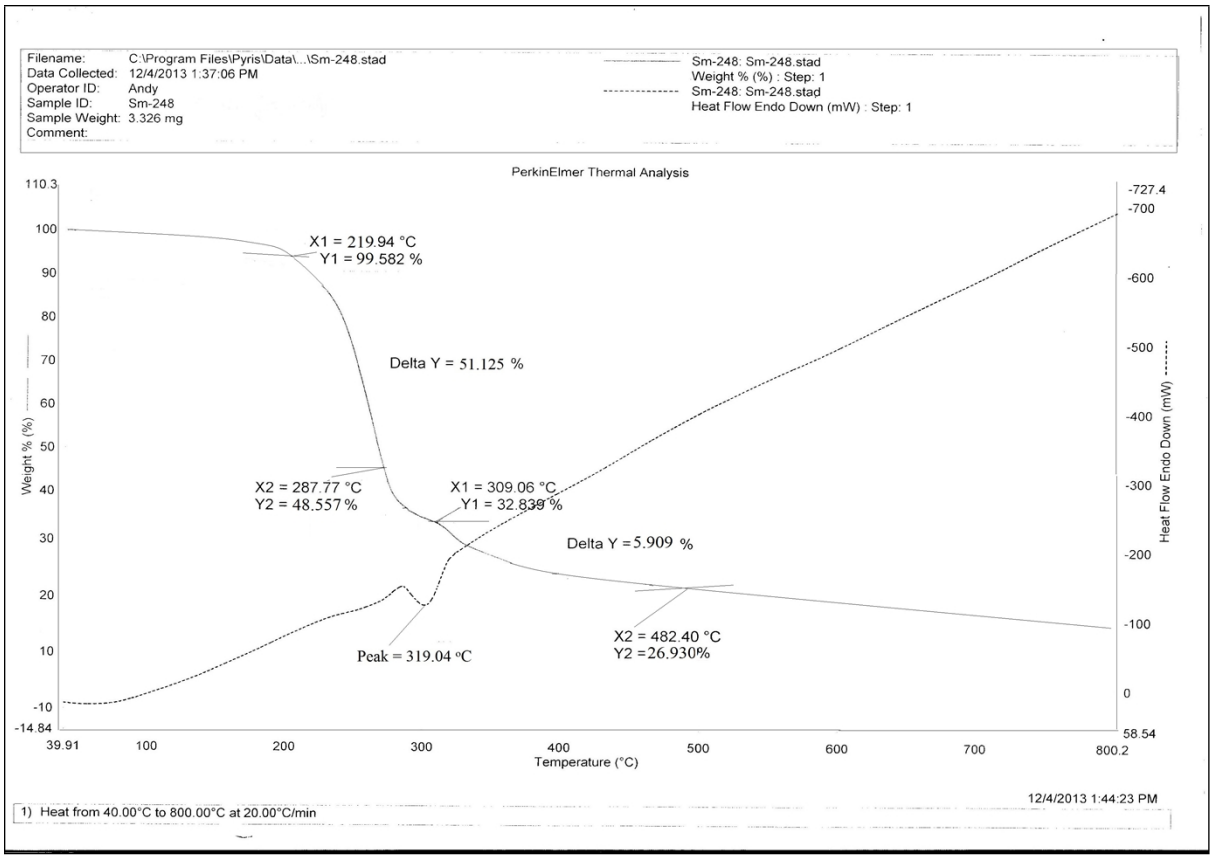
Fig. S2 Theoretical IR spectra for L-Val and its metal complexes in gas and in aqueous phase



TG/DTA curve for $Ni(L\text{-}Val)_2$ (Solid state technique)

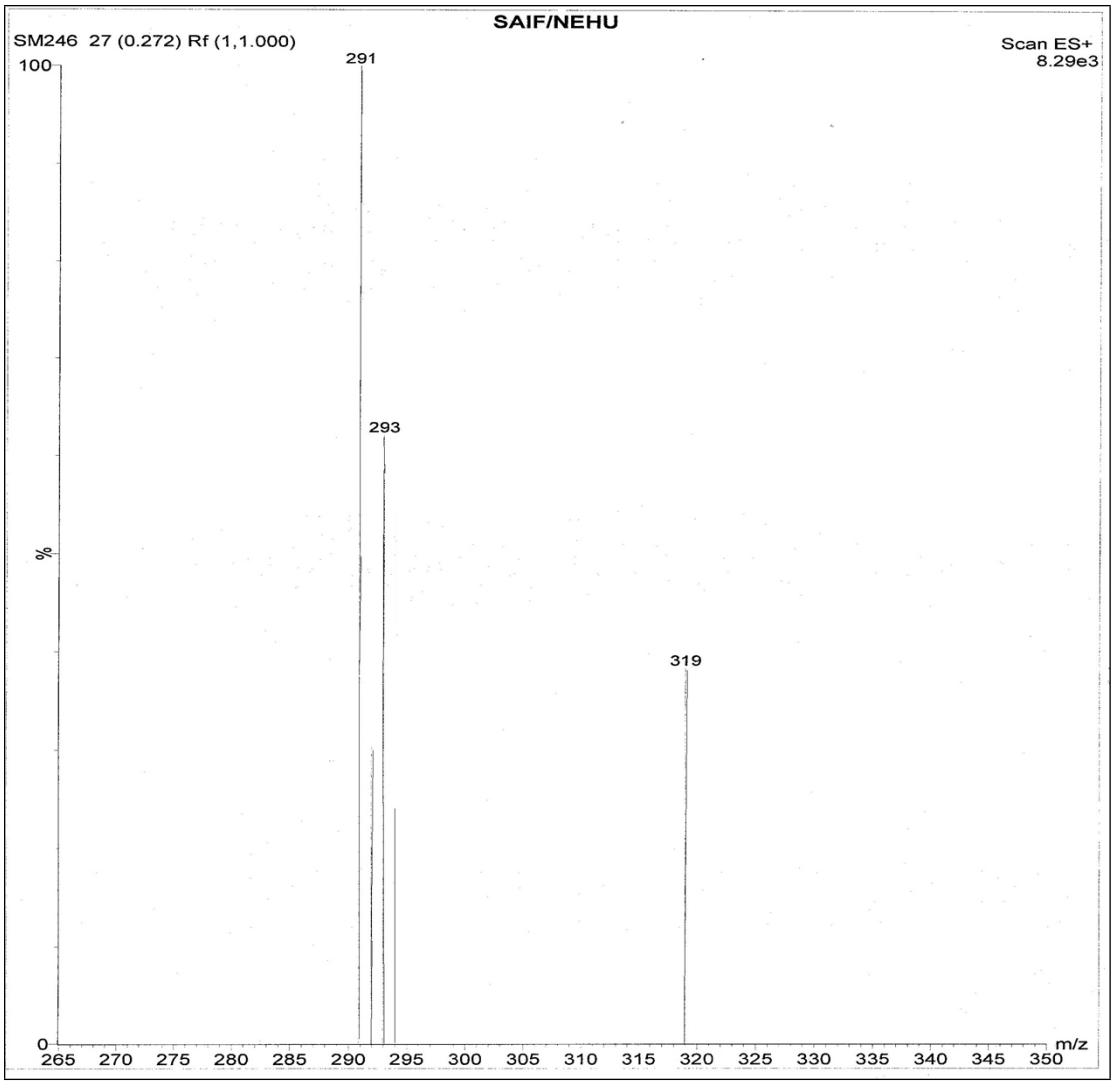


TG/DTA curve for $Cu(L\text{-}Val)_2$ (Solid state technique)

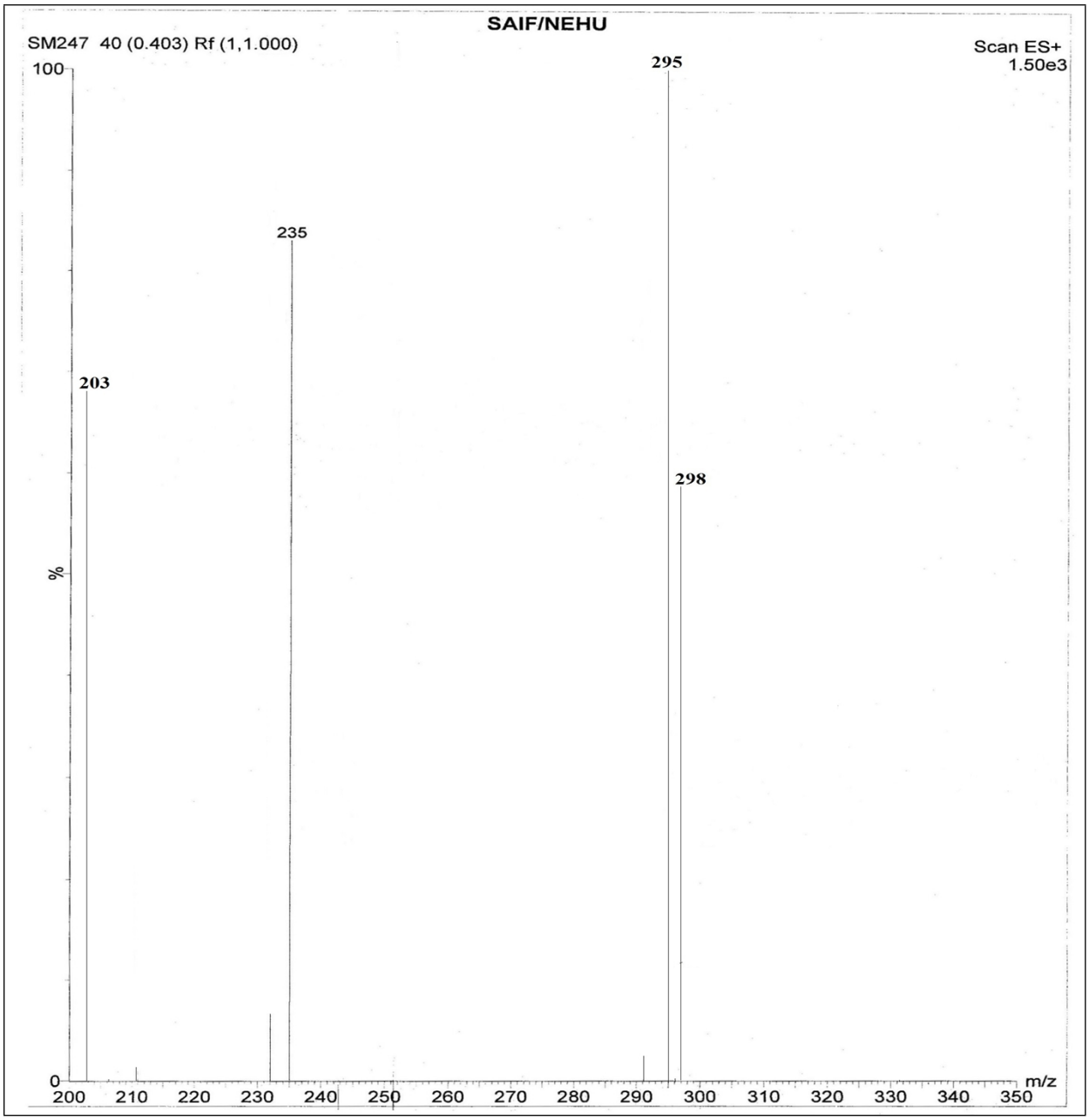


TG/DTA curve for $Zn(L\text{-}Val)_2$ (Solid state technique)

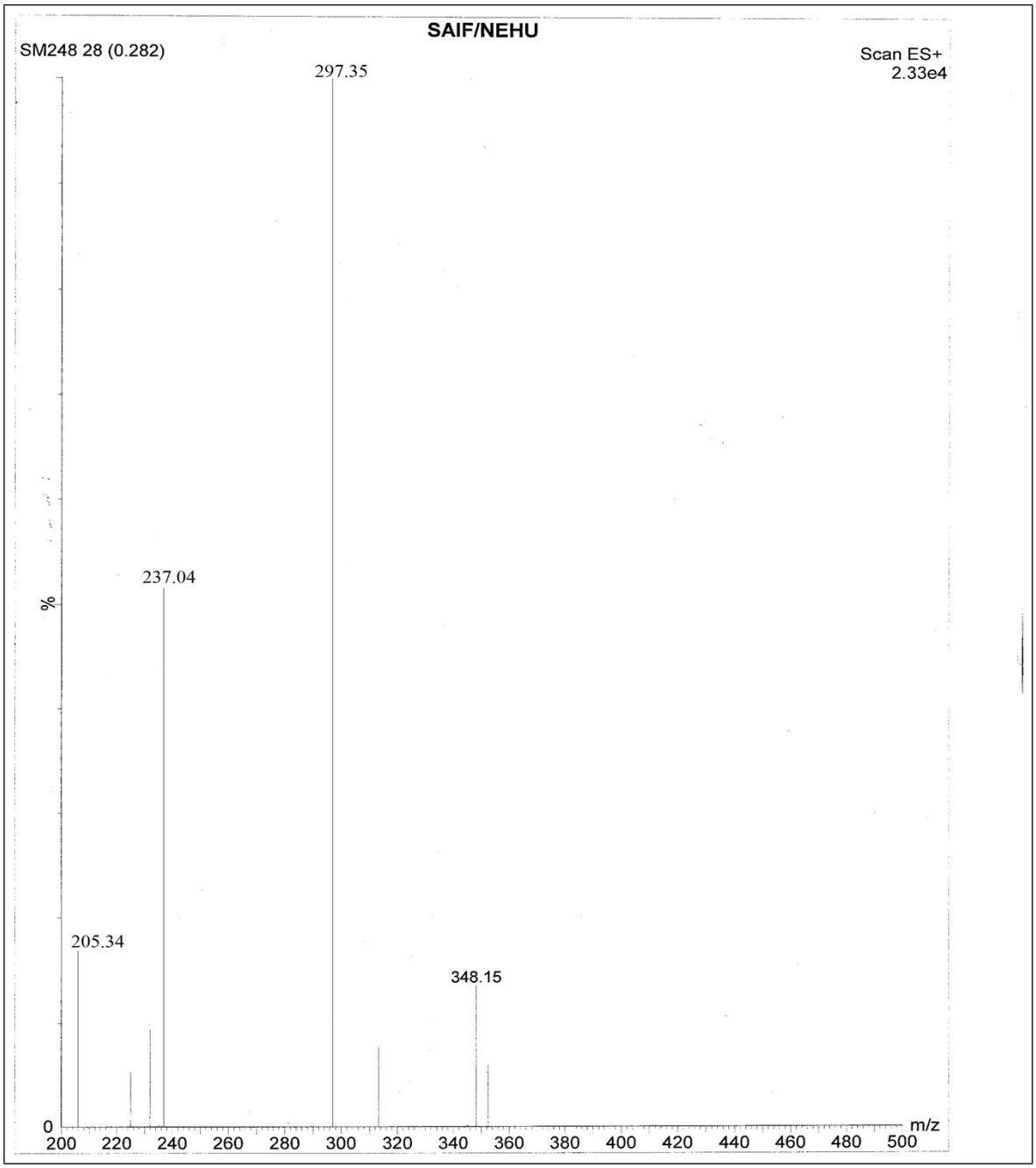
Fig. S3 Experimental TG/DTA Curves of the metal complexes prepared in solid state



Mass spectrum of the complex $Ni(L\text{-}Val)_2$ in DMSO solution.



Mass spectrum of the complex $Cu(L\text{-}Val)_2$ in DMSO solution.



Mass spectrum of the complex $Zn(L\text{-}Val)_2$ in DMSO solution.

Fig. S4 Mass spectrum of the metal complexes prepared by solid state technique.

► Summary of EDA results of kitaura-morokuma analysis for $Ni(Val)_2$ and $Zn(Val)_2$

A) $Ni(Val)_2$

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          RESULTS OF KITAURA-MOROKUMA ANALYSIS
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                    HARTREE    KCAL/MOLE
ELECTROSTATIC ENERGY             ES=-2157.821820   ********
EXCHANGE REPULSION ENERGY        EX=    6.556164    4114.06
POLARIZATION ENERGY              PL= 2157.821820   ********
CHARGE TRANSFER ENERGY           CT= 4323.883938   ********
HIGH ORDER COUPLING ENERGY      MIX=-4330.440102   ********
TOTAL INTERACTION ENERGY,   DELTA-E=    0.000000       0.00

                   DECOMPOSITION OF CT
CHARGE TRANSFER ENERGY, MON=  1  CT= 2161.941969   ********
CHARGE TRANSFER ENERGY, MON=  2  CT= 2161.941969   ********

                   DECOMPOSITION OF PL
EPL,                    MON=  1  PL= 2157.821820   ********
EPL,                    MON=  2  PL= 2157.821820   ********
HIGH ORDER COUPLING FOR PL,    PMIX=-2157.821820   ********
           ... END OF MOROKUMA DECOMPOSITION ...
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B) $Zn(Val)_2$

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          RESULTS OF KITAURA-MOROKUMA ANALYSIS
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                    HARTREE    KCAL/MOLE
ELECTROSTATIC ENERGY             ES=-1959.914255   ********
EXCHANGE REPULSION ENERGY        EX=    0.368053     230.96
POLARIZATION ENERGY              PL= 1959.914255   ********
CHARGE TRANSFER ENERGY           CT= 3922.034703   ********
HIGH ORDER COUPLING ENERGY      MIX=-3922.402756   ********
TOTAL INTERACTION ENERGY,   DELTA-E=    0.000000       0.00

                   DECOMPOSITION OF CT
CHARGE TRANSFER ENERGY, MON=  1  CT= 1961.017352   ********
CHARGE TRANSFER ENERGY, MON=  2  CT= 1961.017352   ********

                   DECOMPOSITION OF PL
EPL,                    MON=  1  PL= 1959.914255   ********
EPL,                    MON=  2  PL= 1959.914255   ********
HIGH ORDER COUPLING FOR PL,    PMIX=-1959.914255   ********
           ... END OF MOROKUMA DECOMPOSITION ...
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► Cartesian coordinates of optimized structures

For L-Val in gas phase

1	7	0	-0.376772	-1.814289	0.086085
2	6	0	-0.095392	-0.386184	0.338563
3	1	0	0.007043	-0.282260	1.426747
4	6	0	1.188766	0.189200	-0.317909
5	6	0	-1.380953	0.409791	-0.015622
6	1	0	0.977305	0.334615	-1.385371
7	8	0	-2.488828	-0.347661	-0.024159
8	8	0	-1.414359	1.592308	-0.233529
9	1	0	-0.173839	-2.068205	-0.876778
10	1	0	0.175058	-2.418818	0.682529
11	6	0	2.370161	-0.785067	-0.187122
12	6	0	1.574792	1.549417	0.285726
13	1	0	2.199570	-1.736182	-0.697045
14	1	0	3.268439	-0.340234	-0.622641
15	1	0	2.590205	-0.999128	0.865218
16	1	0	1.804612	1.442194	1.352385
17	1	0	2.471271	1.937864	-0.205583
18	1	0	0.774747	2.278454	0.177016
19	1	0	-2.175757	-1.268400	0.120611

For L-Val in aqueous phase

1	7	0	0.274115	1.848538	0.133428
2	6	0	0.068122	0.378081	0.442718
3	1	0	-0.110413	0.278697	1.513233
4	6	0	-1.144647	-0.152220	-0.356409
5	6	0	1.434465	-0.293245	0.071357
6	1	0	-0.980179	0.117694	-1.407751
7	8	0	2.134365	0.365528	-0.749030
8	8	0	1.689464	-1.384066	0.608279
9	1	0	-0.530164	2.302472	-0.298729
10	1	0	0.536870	2.389794	0.956975
11	6	0	-2.454291	0.500067	0.120269
12	6	0	-1.266995	-1.679834	-0.277514
13	1	0	-2.452407	1.591912	0.050534
14	1	0	-3.289062	0.146795	-0.489481
15	1	0	-2.659540	0.234060	1.161707
16	1	0	-1.402922	-2.009339	0.756800
17	1	0	-2.140416	-2.001350	-0.850313
18	1	0	-0.387350	-2.182963	-0.677568
19	1	0	1.086225	1.823674	-0.525925

For $Ni(L\text{-}Val)_2$ in gas phase

1	7	0	-1.678382	0.928648	-0.209709
2	6	0	-2.749549	0.021183	0.312236
3	1	0	-2.693886	0.093173	1.405009
4	6	0	-4.174767	0.408396	-0.139169
5	6	0	-2.301532	-1.428269	-0.041015
6	1	0	-4.278296	0.112860	-1.191493
7	8	0	-1.005918	-1.548544	-0.196475
8	7	0	1.678390	-0.928584	-0.209908
9	6	0	2.749549	-0.021203	0.312199
10	1	0	2.693786	-0.093258	1.404964
11	6	0	4.174757	-0.408443	-0.139129
12	6	0	2.301555	1.428276	-0.041003
13	1	0	4.278306	-0.112974	-1.191473
14	8	0	1.005912	1.548585	-0.196228
15	28	0	-0.000004	0.000021	-0.189096
16	8	0	3.091490	2.345494	-0.123032
17	8	0	-3.091460	-2.345511	-0.122886
18	1	0	1.869440	-1.183503	-1.178642
19	1	0	1.614908	-1.801242	0.308642
20	1	0	-1.869428	1.183828	-1.178372
21	1	0	-1.614889	1.801174	0.309065
22	6	0	-4.419033	1.923270	-0.029706
23	6	0	-5.235463	-0.348051	0.676085
24	6	0	5.235484	0.348011	0.676106
25	6	0	4.418991	-1.923329	-0.029612
26	1	0	-3.770927	2.516726	-0.680882
27	1	0	-5.449052	2.154718	-0.311391
28	1	0	-4.277075	2.271994	0.999623
29	1	0	-5.186387	-0.056695	1.731686
30	1	0	-6.235506	-0.097879	0.311487
31	1	0	-5.095211	-1.424718	0.604967
32	1	0	6.235509	0.097909	0.311404
33	1	0	5.095205	1.424679	0.605047
34	1	0	5.186501	0.056560	1.731680
35	1	0	5.449036	-2.154801	-0.311188
36	1	0	4.276936	-2.272026	0.999708
37	1	0	3.770939	-2.516799	-0.680835

For $Ni(L\text{-}Val)_2$ in aqueous phase

1	7	0	1.690180	-0.920962	-0.222940
2	6	0	2.754005	-0.014911	0.308736
3	1	0	2.686091	-0.085681	1.400307
4	6	0	4.188786	-0.398127	-0.123582
5	6	0	2.307812	1.425125	-0.043490
6	1	0	4.319213	-0.075967	-1.164029
7	8	0	1.023644	1.556299	-0.220688
8	7	0	-1.690208	0.920914	-0.222832
9	6	0	-2.754042	0.014786	0.308690
10	1	0	-2.686123	0.085384	1.400272

11	6	0	-4.188801	0.398142	-0.123569
12	6	0	-2.307854	-1.425192	-0.043801
13	1	0	-4.319350	0.075874	-1.163969
14	8	0	-1.023676	-1.556343	-0.220944
15	28	0	-0.000014	-0.000024	-0.207831
16	8	0	-3.095784	-2.361206	-0.110615
17	8	0	3.095780	2.361105	-0.110330
18	1	0	-1.888502	1.174818	-1.190514
19	1	0	-1.645583	1.791311	0.301054
20	1	0	1.888485	-1.174717	-1.190659
21	1	0	1.645547	-1.791441	0.300810
22	6	0	4.421763	-1.916892	-0.055163
23	6	0	5.234553	0.319715	0.744494
24	6	0	-5.234630	-0.319402	0.744679
25	6	0	-4.421519	1.916954	-0.055333
26	1	0	3.788210	-2.479434	-0.744911
27	1	0	5.458759	-2.140535	-0.317353
28	1	0	4.247297	-2.296992	0.957260
29	1	0	5.156741	-0.010914	1.786174
30	1	0	6.240925	0.075729	0.393538
31	1	0	5.108144	1.400506	0.713793
32	1	0	-6.240984	-0.075257	0.393780
33	1	0	-5.108434	-1.400219	0.714095
34	1	0	-5.156667	0.011335	1.786315
35	1	0	-5.458501	2.140737	-0.317457
36	1	0	-4.246892	2.297157	0.957023
37	1	0	-3.787933	2.479297	-0.745214

For $Cu(L\text{-}Val)_2$ in gas phase

1	7	0	-1.785052	0.964430	-0.226556
2	6	0	-2.826814	0.030742	0.299858
3	1	0	-2.742162	0.080758	1.392649
4	6	0	-4.273360	0.401510	-0.098104
5	6	0	-2.382436	-1.417352	-0.090954
6	1	0	-4.415435	0.094428	-1.142138
7	8	0	-1.089242	-1.571052	-0.186865
8	7	0	1.785026	-0.964471	-0.226125
9	6	0	2.826843	-0.030704	0.300012
10	1	0	2.742394	-0.080608	1.392827
11	6	0	4.273312	-0.401513	-0.098162
12	6	0	2.382416	1.417356	-0.090823
13	1	0	4.415194	-0.094519	-1.142250
14	8	0	1.089215	1.571050	-0.186624
15	8	0	3.198434	2.303635	-0.248024
16	8	0	-3.198469	-2.303628	-0.248057
17	1	0	1.980825	-1.207792	-1.195842
18	1	0	1.749079	-1.841078	0.286760

19	1	0	-1.980879	1.207371	-1.196363
20	1	0	-1.749213	1.841223	0.286020
21	6	0	-4.534108	1.913715	0.009018
22	6	0	-5.292148	-0.359874	0.765189
23	6	0	5.292268	0.359944	0.764887
24	6	0	4.534097	-1.913711	0.009029
25	1	0	-3.921570	2.509626	-0.673445
26	1	0	-5.578028	2.128438	-0.232139
27	1	0	-4.355858	2.274840	1.028600
28	1	0	-5.197807	-0.066486	1.817356
29	1	0	-6.309585	-0.117355	0.446215
30	1	0	-5.149446	-1.435681	0.687252
31	1	0	6.309633	0.117626	0.445508
32	1	0	5.149427	1.435745	0.687067
33	1	0	5.198340	0.066364	1.817027
34	1	0	5.578002	-2.128418	-0.232222
35	1	0	4.355981	-2.274798	1.028644
36	1	0	3.921520	-2.509713	-0.673328
37	29	0	-0.000005	-0.000014	-0.183537

For $Cu(L\text{-}Val)_2$ in aqueous phase

1	7	0	1.781679	-0.949353	-0.213375
2	6	0	2.827454	-0.018336	0.301897
3	1	0	2.740629	-0.053580	1.394302
4	6	0	4.276328	-0.401132	-0.086555
5	6	0	2.394943	1.419937	-0.099047
6	1	0	4.439029	-0.074794	-1.120823
7	8	0	1.115264	1.589578	-0.230753
8	7	0	-1.781639	0.949443	-0.213794
9	6	0	-2.827406	0.018566	0.301747
10	1	0	-2.740530	0.054034	1.394142
11	6	0	-4.276320	0.401191	-0.086719
12	6	0	-2.394917	-1.419764	-0.098957
13	1	0	-4.438834	0.075196	-1.121123
14	8	0	-1.115211	-1.589495	-0.230280
15	8	0	-3.217396	-2.320902	-0.235981
16	8	0	3.217475	2.320875	-0.237054
17	1	0	-1.977659	1.209959	-1.179351
18	1	0	-1.756823	1.814496	0.318943
19	1	0	1.977742	-1.210191	-1.178836
20	1	0	1.756830	-1.814235	0.319642
21	6	0	4.515301	-1.918768	-0.016165
22	6	0	5.292060	0.316644	0.817115
23	6	0	-5.291942	-0.317234	0.816553
24	6	0	-4.515710	1.918738	-0.015759
25	1	0	3.904832	-2.481730	-0.725997
26	1	0	5.560839	-2.135711	-0.249043
27	1	0	4.314783	-2.304700	0.989338
28	1	0	5.182712	-0.019606	1.854316
29	1	0	6.310729	0.079701	0.497842

30	1	0	5.161746	1.397072	0.787010
31	1	0	-6.310646	-0.080504	0.497235
32	1	0	-5.161277	-1.397613	0.786067
33	1	0	-5.182834	0.018664	1.853893
34	1	0	-5.561282	2.135485	-0.248662
35	1	0	-4.315409	2.304335	0.989917
36	1	0	-3.905327	2.482147	-0.725309
37	29	0	0.000023	0.000050	-0.195705

For $Zn(L\text{-}Val)_2$ in gas phase

1	7	0	1.754000	-0.739319	0.693850
2	6	0	2.780876	0.349786	0.596387
3	1	0	2.759107	0.873967	1.557803
4	6	0	4.215558	-0.168571	0.363799
5	6	0	2.370221	1.434114	-0.455219
6	8	0	1.156589	1.372987	-0.916871
7	7	0	-1.753834	0.739462	0.693445
8	6	0	-2.780887	-0.349522	0.596449
9	1	0	-2.759090	-0.873385	1.558040
10	6	0	-4.215517	0.169013	0.363888
11	6	0	-2.370477	-1.434260	-0.454800
12	8	0	-1.156703	-1.373782	-0.916178
13	8	0	-3.195124	-2.283439	-0.735831
14	8	0	3.194603	2.283532	-0.736290
15	30	0	0.000037	-0.000310	-0.226236
16	1	0	-2.028527	1.531643	0.114099
17	1	0	-1.696226	1.098889	1.641613
18	1	0	2.028808	-1.531709	0.114844
19	1	0	1.696446	-1.098339	1.642174
20	1	0	4.822229	0.737317	0.292155
21	1	0	-4.822386	-0.736771	0.292617
22	6	0	4.358430	-0.924473	-0.965507
23	6	0	4.722697	-1.003694	1.547440
24	6	0	-4.358438	0.924510	-0.965637
25	6	0	-4.722295	1.004638	1.547332
26	1	0	-3.797279	1.867590	-0.978443
27	1	0	-4.027057	0.315183	-1.809254
28	1	0	-5.404985	1.187505	-1.137813
29	1	0	-4.163127	1.940589	1.662810
30	1	0	-5.770803	1.277581	1.403008
31	1	0	-4.652221	0.450563	2.488807
32	1	0	5.405011	-1.187267	-1.137777
33	1	0	3.797494	-1.867689	-0.977923
34	1	0	4.026754	-0.315511	-1.809277
35	1	0	5.771216	-1.276527	1.402996
36	1	0	4.652721	-0.449279	2.488721
37	1	0	4.163700	-1.939690	1.663383

For $Zn(L\text{-}Val)_2$ in aqueous phase

1	7	0	1.750779	-0.666365	0.711519
2	6	0	2.798658	0.383466	0.572013
3	1	0	2.750940	0.987771	1.483389
4	6	0	4.232773	-0.181205	0.452404
5	6	0	2.447526	1.377618	-0.571221
6	8	0	1.262332	1.314121	-1.072841
7	7	0	-1.750558	0.666733	0.711520
8	6	0	-2.798704	-0.382974	0.573128
9	1	0	-2.751174	-0.986282	1.485174
10	6	0	-4.232641	0.182017	0.452828
11	6	0	-2.447853	-1.378367	-0.569118
12	8	0	-1.262882	-1.315234	-1.071336
13	8	0	-3.301227	-2.204150	-0.902084
14	8	0	3.300850	2.202954	-0.905425
15	30	0	-0.000111	-0.000313	-0.265299
16	1	0	-2.037247	1.524983	0.245740
17	1	0	-1.607706	0.908610	1.687350
18	1	0	2.037555	-1.524915	0.246357
19	1	0	1.608219	-0.907475	1.687584
20	1	0	4.873706	0.697948	0.351469
21	1	0	-4.874078	-0.697091	0.354698
22	6	0	4.429698	-1.047768	-0.800813
23	6	0	4.649560	-0.933472	1.724235
24	6	0	-4.429882	1.045209	-0.802664
25	6	0	-4.648295	0.938040	1.722814
26	1	0	-3.850093	1.974505	-0.766739
27	1	0	-4.152595	0.506991	-1.712525
28	1	0	-5.479441	1.335935	-0.894404
29	1	0	-4.049109	1.841901	1.874277
30	1	0	-5.693972	1.249393	1.654129
31	1	0	-4.542363	0.310411	2.612610
32	1	0	5.479422	-1.337882	-0.892583
33	1	0	3.850755	-1.977463	-0.761735
34	1	0	4.151199	-0.512407	-1.711998
35	1	0	5.695297	-1.244667	1.655717
36	1	0	4.544065	-0.303280	2.612270
37	1	0	4.050780	-1.837095	1.878775