

Supplementary Data

This supplementary data is a part of a paper entitled “Synthesis and Antibacterial Activity of Azomethine Ligand and Their Metal Complexes: A Combined Experimental and Theoretical Study”.

Table S1. Cartesian coordinated for VOL complex

C	1.272739	-8.95117	0.669916
C	0.378947	-9.45143	-0.22054
C	-0.55549	-8.60426	-0.82781
C	-0.56522	-7.24541	-0.51865
C	0.363201	-6.74534	0.407095
C	1.262672	-7.58317	0.98916
C	-1.47302	-9.11397	-1.74688
C	-1.48918	-6.38256	-1.12936
C	-2.43127	-6.89157	-2.03507
C	-2.41415	-8.26254	-2.3543
H	-1.46116	-10.1545	-1.98505
H	1.989149	-9.60297	1.126378
H	0.388275	-10.4951	-0.45705
H	0.361304	-5.70572	0.659025
H	1.970879	-7.19955	1.694769
C	-1.42129	-4.88687	-0.76467
H	-2.42219	-4.88526	-1.16411
H	-0.87503	-5.30127	0.061346
C	-2.10272	-4.11693	0.388127
N	-2.50691	-4.67593	1.527182
C	-2.47542	-2.50364	1.828729
N	-3.14871	-3.68453	2.297323
N	-2.33201	-2.65304	0.394937
N	-1.23974	-1.89275	-0.08105
C	0.94241	-2.88499	-0.83383
C	1.587989	-3.36704	-1.97784
C	1.61517	-2.85693	0.395513
C	2.858089	-3.92954	-1.89068
H	1.091231	-3.31194	-2.92572
C	2.899628	-3.42856	0.483799
H	1.15824	-2.41672	1.260834
C	3.494614	-4.00459	-0.65322
H	3.338317	-4.30337	-2.77041
H	3.419091	-3.43302	1.419848
C	-0.51829	-2.43627	-1.01378
H	-0.979	-2.59855	-1.96469
O	4.753896	-4.67787	-0.56022
C	5.810718	-5.61779	-0.81649

H	6.139512	-5.52071	-1.83163
H	6.628929	-5.42546	-0.15845
H	5.448534	-6.61318	-0.65635
H	-3.11517	-8.65701	-3.05937
H	-3.15602	-6.24309	-2.48304
S	-1.86406	-1.26851	2.544346
S	-3.08499	0.526407	0.480295
C	-2.92216	1.948908	0.010483
N	-3.94589	2.70945	-0.60599
N	-1.64595	2.483092	-0.42772
N	-3.35512	3.982278	-0.53574
C	-2.05189	4.182112	-0.71311
N	-0.61541	1.60377	0.23901
C	-1.77209	5.683839	-0.55636
C	0.599551	1.97952	0.466446
C	-2.22277	6.999556	0.093163
H	-1.84895	6.149147	-1.5174
H	-0.78633	5.844113	-0.16537
C	1.920825	2.76924	0.627406
H	1.277935	1.226676	0.822952
C	-2.32415	8.181699	-0.66692
C	-2.56138	7.019475	1.456099
C	2.266319	3.599291	-0.44292
C	2.773003	2.688626	1.752625
C	-2.79117	9.353439	-0.06225
C	-1.97792	8.196805	-2.03122
C	-2.99566	8.206543	2.060171
H	-2.48334	6.120876	2.037925
C	3.437525	4.36111	-0.41863
H	1.61756	3.646924	-1.28952
C	3.969206	3.438273	1.760494
H	2.525736	2.062654	2.591729
C	-2.96141	10.50773	-0.82789
C	-3.09755	9.377981	1.302769
C	-2.13158	9.339266	-2.75095
H	-1.59741	7.311725	-2.49878
H	-3.25008	8.216368	3.101555
C	4.296884	4.278149	0.676613
H	3.675286	4.998772	-1.2434

H	4.636085	3.366752	2.592704
C	-2.63952	10.50285	-2.14608
H	-3.34594	11.39971	-0.37872
H	-3.40726	10.29136	1.764164
H	-1.86752	9.355891	-3.78901
O	5.50951	5.050666	0.697191
H	-2.77546	11.39085	-2.72746
C	6.671422	5.77632	0.278036
H	6.373125	6.616304	-0.31688
H	7.208149	6.12629	1.139323
H	7.298841	5.132196	-0.29629
V	-1.05552	-0.20732	0.821262
O	0.524379	-0.20178	1.231423

Table S2. Cartesian coordinated for CrL complex

C	-0.37962	5.738825	9.038792
C	0.253356	5.198548	7.966993
C	0.594882	6.008334	6.877074
C	0.273734	7.370842	6.90002
C	-0.38329	7.907451	8.013491
C	-0.70174	7.106801	9.061188
C	1.249388	5.458452	5.768075
C	0.60814	8.191133	5.813217
C	1.270538	7.643997	4.705556
C	1.59178	6.278111	4.684289
H	1.48823	4.414398	5.748116
H	-0.63713	5.118374	9.871691
H	0.49261	4.154667	7.95523
H	-0.63634	8.947581	8.037182
H	-1.20101	7.520952	9.911626
C	0.236728	9.687218	5.826475
H	-0.71523	9.307983	5.509527
H	1.21643	9.806651	5.416695
C	-0.10688	10.81672	4.840954
N	-0.63322	10.60837	3.655029
C	-0.96873	12.66442	4.126482
N	-1.14008	11.83901	3.158895
N	0.076749	12.25655	5.030041
N	-0.08014	12.90477	6.305221
C	2.183616	12.11325	6.789284
C	3.275725	12.07317	7.67053
C	2.275201	11.50291	5.532739
C	4.464386	11.43335	7.279434
H	3.207693	12.52907	8.636989

C	3.45422	10.85523	5.149507
H	1.441488	11.53222	4.865154
C	4.550829	10.82417	6.018735
H	5.304921	11.40952	7.941953
H	3.517133	10.3852	4.192204
C	0.876129	12.83295	7.181084
H	0.767088	13.27479	8.152712
O	5.757748	10.17295	5.62503
C	6.867348	10.84383	6.226019
H	6.762394	10.82591	7.291025
H	7.776239	10.35047	5.951035
H	6.894324	11.8569	5.88714
H	2.095883	5.861024	3.838862
H	1.528652	8.268216	3.875278
S	-1.75442	13.9212	4.479044
S	-2.82951	12.11447	6.562263
C	-4.27207	12.64408	6.528017
N	-5.43697	12.09069	6.697049
N	-4.38202	14.03103	6.289191
N	-6.36383	13.17449	6.903465
C	-5.68344	14.29378	6.835306
N	-3.29295	14.71174	6.848375
C	-7.05625	14.86074	7.228091
C	-3.54854	15.82859	7.453535
C	-8.42886	15.42761	7.62082
H	-7.06773	15.14645	6.195106
H	-7.18001	13.88216	7.643163
C	-3.44096	17.13919	8.235562
H	-4.61588	15.74592	7.442709
C	-8.88243	16.53194	6.898969
C	-9.20612	14.89966	8.654871
C	-3.95899	17.13989	9.533359
C	-2.87215	18.30366	7.703925
C	-10.0988	17.13564	7.209466
C	-8.09711	17.04123	5.860526
C	-10.4368	15.50497	8.972428
H	-8.86942	14.04312	9.201369
C	-3.96855	18.31124	10.28894
H	-4.35147	16.23425	9.94831
C	-2.8934	19.49093	8.460494
H	-2.43599	18.29492	6.729116
C	-10.5196	18.24867	6.472124
C	-10.8828	16.62461	8.251013
C	-8.52318	18.10924	5.149658

H	-7.15799	16.58445	5.626858
H	-11.0348	15.11121	9.764247
C	-3.47073	19.49583	9.742189
H	-4.36121	18.30215	11.28582
H	-2.47365	20.39209	8.060843
C	-9.74678	18.72013	5.458055
H	-11.4447	18.72706	6.705901
H	-11.8191	17.08745	8.499549
H	-7.92116	18.49013	4.350052
O	-3.56594	20.70828	10.49349
H	-10.0741	19.56448	4.891173
C	-4.74078	20.65526	11.31594
H	-4.65118	19.85206	12.01706
H	-4.8501	21.57856	11.84322
H	-5.60221	20.49399	10.69993
Cr	-1.63246	13.8939	6.602209
Cl	-0.31708	15.55639	6.659238
Cl	-1.35257	13.75557	8.700686

C	2.03224	11.33708	4.966594
C	2.357075	11.74815	3.668674
C	2.891904	11.63241	6.034985
C	3.568928	12.39376	3.4163
H	1.674244	11.56309	2.865782
C	4.122372	12.2687	5.787481
H	2.616316	11.36968	7.032353
C	4.469899	12.62275	4.469445
H	3.809904	12.71141	2.421167
H	4.793059	12.4739	6.597194
C	0.74221	10.55121	5.177624
H	0.875875	9.651273	4.63115
O	5.74504	13.20463	4.179643
C	6.147072	12.78154	2.86395
H	5.451871	13.15255	2.14175
H	7.122697	13.16308	2.648585
H	6.168168	11.71203	2.823837
H	0.498834	4.27418	2.261281
H	-0.05878	6.508626	3.150217
S	-1.89415	10.96702	7.977813
S	-3.08527	12.1085	5.697454
C	-3.7204	13.46821	5.9838
N	-5.08626	13.92303	6.02431
N	-2.86238	14.53472	6.394607
N	-5.04887	14.74448	7.179819
C	-3.86152	15.33279	7.15188
N	-1.74061	13.99966	7.113859
C	-3.77789	16.77478	7.67816
C	-1.27498	14.70793	8.112658
C	-4.86126	17.03991	8.743116
H	-3.94272	17.44619	6.870787
H	-2.80173	16.94012	8.103184
C	-0.37222	15.24039	9.259384
H	-1.87024	15.53236	8.440348
C	-5.41782	18.31901	8.712449
C	-5.29574	16.09562	9.696318
C	-0.87436	16.3166	10.00483
C	0.906777	14.72824	9.556437
C	-6.39011	18.68502	9.631978
C	-4.99232	19.22978	7.733319
C	-6.27295	16.47115	10.64711
H	-4.88932	15.10593	9.70465
C	-0.08654	16.95147	10.96775
H	-1.87923	16.65929	9.83429

Table S3. Cartesian coordinated for MnL complex

C	3.867734	3.828717	6.932043
C	3.366582	3.438702	5.741487
C	2.438174	4.248171	5.068612
C	2.069708	5.494659	5.612944
C	2.603961	5.878117	6.854373
C	3.459897	5.043165	7.5112
C	1.881222	3.8155	3.850619
C	1.185522	6.335375	4.895674
C	0.622584	5.878378	3.686525
C	0.951804	4.619758	3.174449
H	2.164247	2.866871	3.43688
H	4.576174	3.208239	7.437333
H	3.673736	2.503729	5.312611
H	2.342191	6.823451	7.284242
H	3.83148	5.314349	8.47851
C	0.807878	7.767343	5.362745
H	0.017408	7.598365	4.662197
H	1.132708	7.400542	6.322306
C	-0.37422	8.310438	6.206708
N	-0.87032	7.562957	7.200571
C	-1.75738	9.589785	7.308202
N	-2.04399	8.219034	7.676651
N	-1.15273	9.552362	6.040453
N	-0.37026	10.70206	5.813863

C	1.709082	15.37394	10.52811
H	1.270541	13.85901	9.049415
C	-6.91204	19.9858	9.588471
C	-6.82806	17.76293	10.59652
C	-5.52561	20.46773	7.683995
H	-4.24022	18.94127	7.024661
H	-6.58896	15.77865	11.40846
C	1.215631	16.52019	11.20174
H	-0.4817	17.77398	11.52593
H	2.69148	14.99445	10.74632
C	-6.49234	20.8548	8.629282
H	-7.63786	20.29782	10.31248

H	-7.58636	18.04482	11.2881
H	-5.21487	21.15519	6.925683
O	2.027932	17.26211	12.12345
H	-6.90179	21.84193	8.594735
C	1.705603	18.65901	11.98594
H	0.663796	18.80371	12.17173
H	2.279104	19.23192	12.68702
H	1.940096	18.97894	10.99008
Mn	-1.07615	12.32412	6.484452
Cl	-0.3701	13.2595	4.670024
Cl	0.72587	12.70598	7.612511

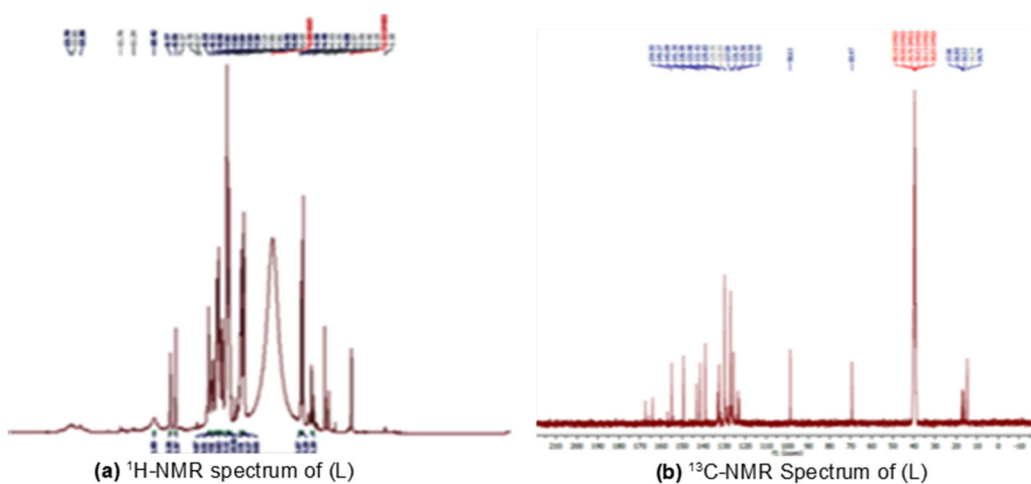


Fig S1. (a) $^1\text{H-}$ and (b) $^{13}\text{C-NMR}$ spectra of ligand (L)

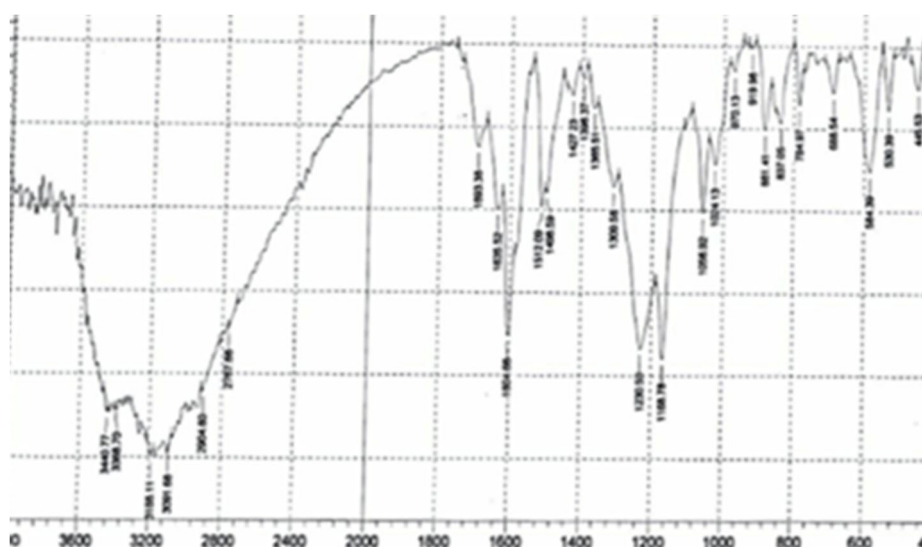


Fig S2. FTIR spectrum of L

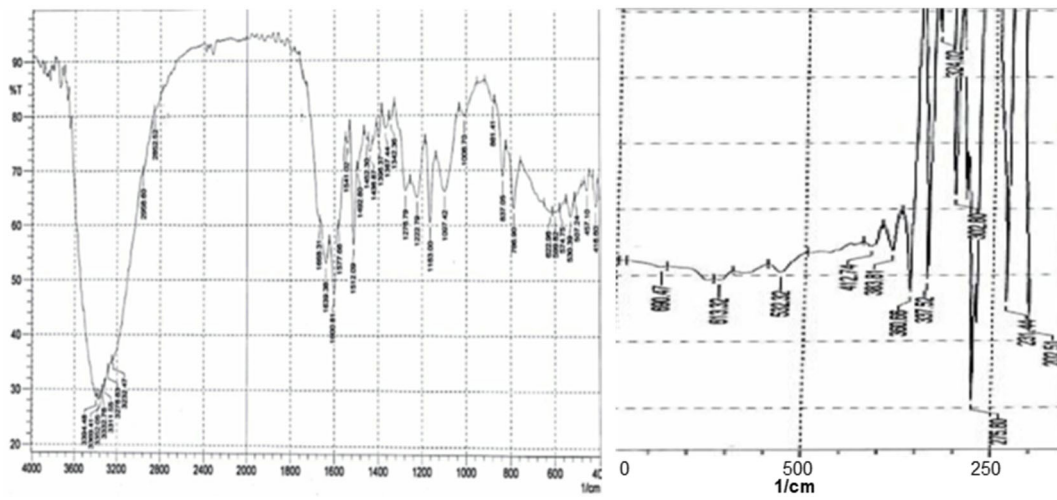


Fig S3. FTIR spectrum for VOL complex

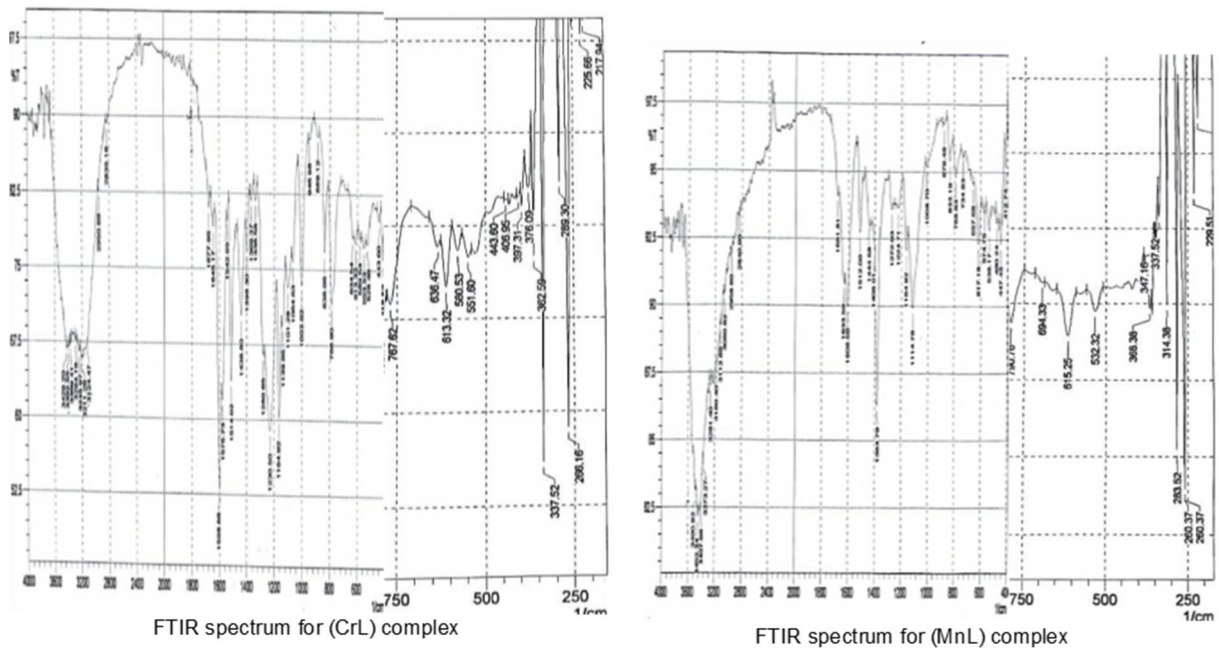


Fig S4. FTIR spectrum for L and its metal complexes

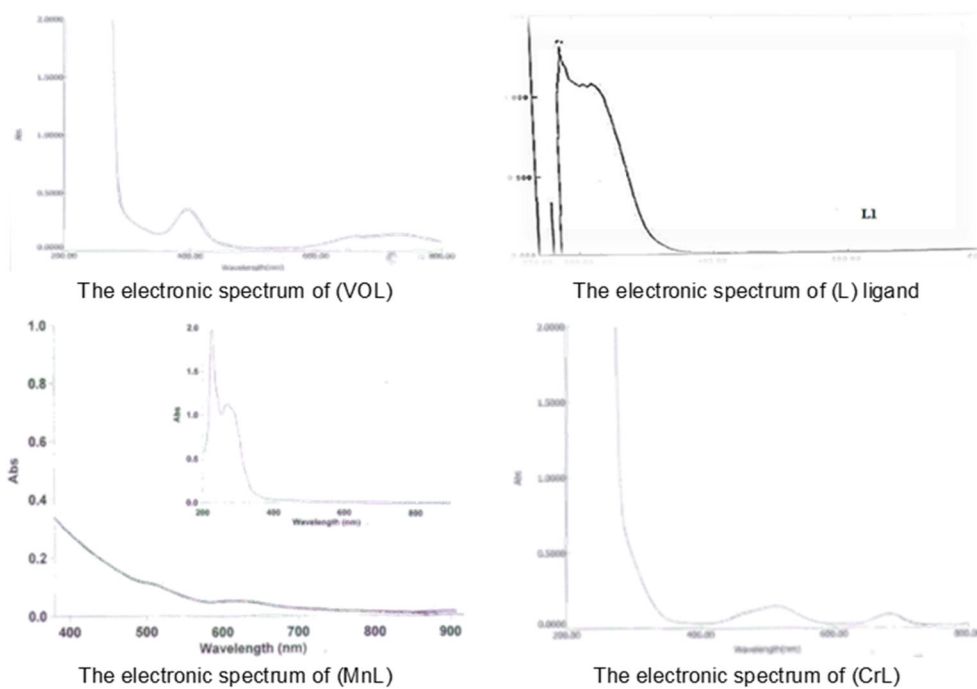


Fig S5. The electronic spectrum of studying compounds

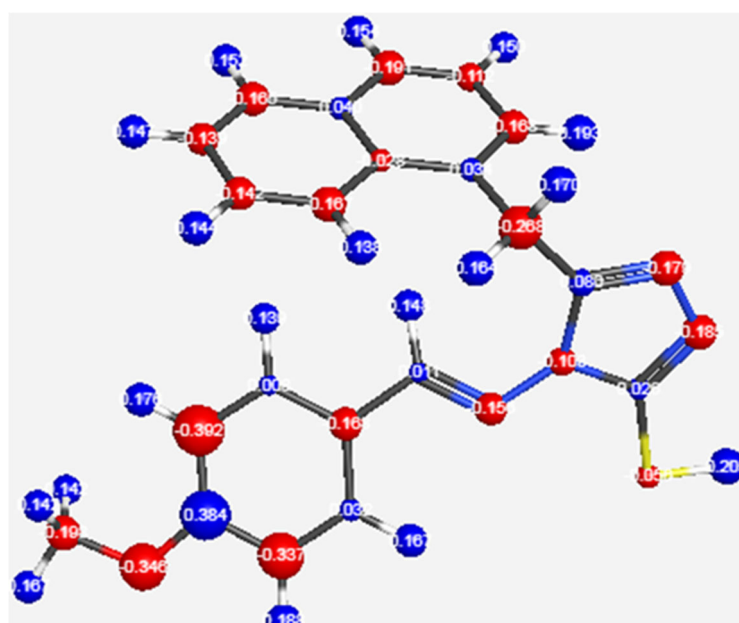


Fig S6. Charge distribution for L