Supplementary Information

A Combined Experimental and Theoretical Investigation on Ligand and Anion Controlled Complex Formation with Unprecedented Structural Features and Photoluminescence Property of Zinc(II) Complexes

Prateeti Chakraborty,[†] Jaydeep Adhikary,[†] Sugata Samanta,[⊥] Daniel Escudero,[‡] Abril C. Castro,[Δ] Marcel Swart, [Δ,Φ] Sanjib Ghosh,[⊥] Antonio Bauzá,[Γ] Antonio Frontera,[*,Γ] Ennio Zangrando*[,§] and Debasis Das,[*,†]

[†]*Department of Chemistry, University of Calcutta, 92 A. P. C. Road, Kolkata-700 009, India, E-mail: dasdebasis2001@yahoo.com*

[‡]*Max-Planck-Institut für Kohlenforschung, Kaiser-Wilhelm-Platz 1, 45470 Mülheim an der Ruhr, Germany,*

[⊥]*Department of Chemistry, Presidency University, Kolkata-700073, India*

[Γ]*Departament de Química, Universitat de les Illes Balears, Crta. de Valldemossa km 7.5, 07122 Palma (Baleares), Spain, E-mail: toni.frontera@uib.es*

[§]*Department of Chemical and Pharmaceutical Sciences, University of Trieste, Via L. Giorgieri 1, 34127 Trieste, Italy, E-mail: ezangrando@units.it*

[Δ] *Institut de Química Computacional i Catàlisi and Departament de Química, Universitat de Girona, Campus de Montilivi, 17071 Girona, Catalonia, Spain*

[Φ]*Institució Catalana de Recerca i Estudis Avançats (ICREA), Pg. Lluís Companys 23, 08010 Barcelona, Catalonia, Spain*

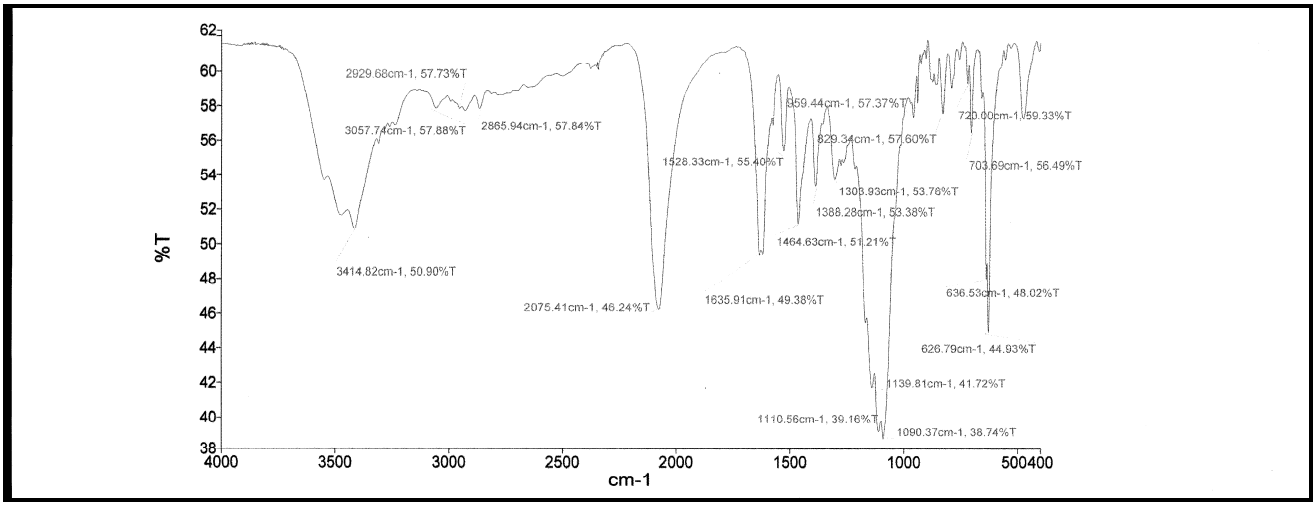

Figure. S1. FT-IR spectrum of complex **1.**

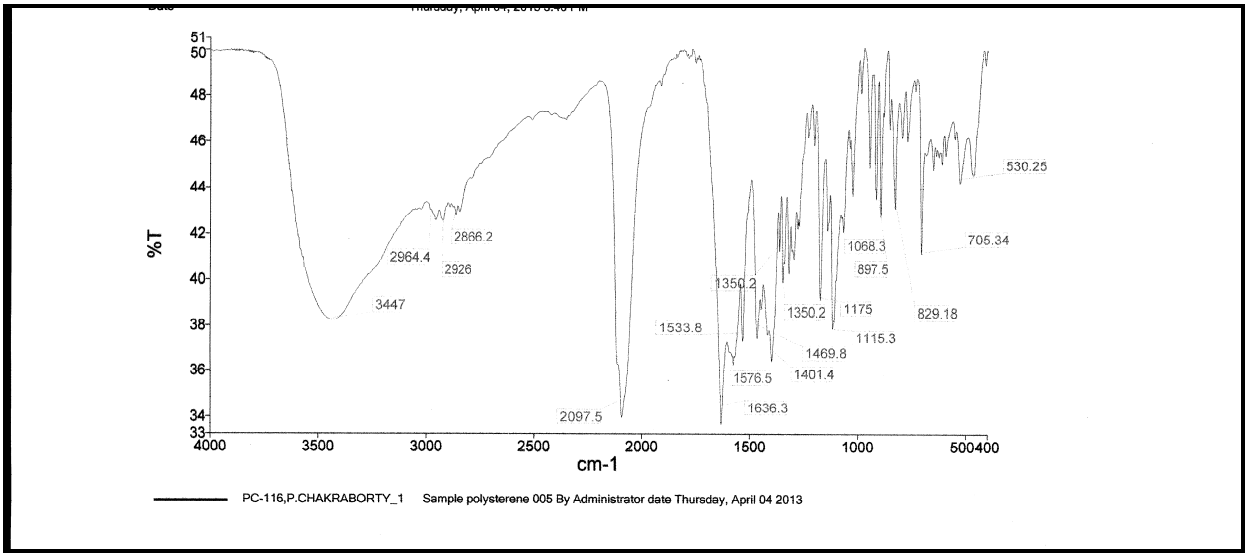

Figure. S2. FT-IR spectrum of complex **2.**

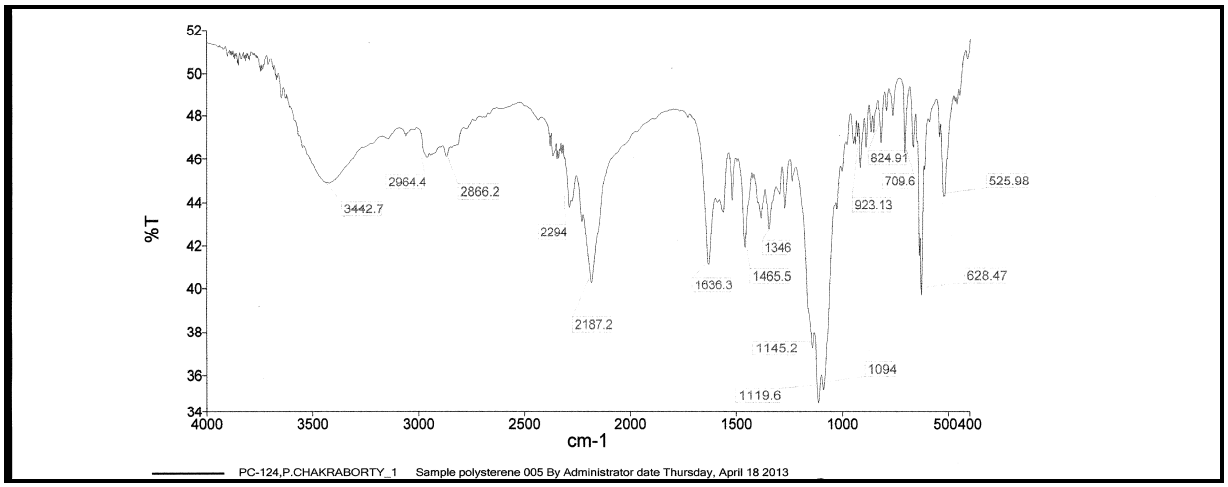

Figure. S3. FT-IR spectrum of complex **3.**

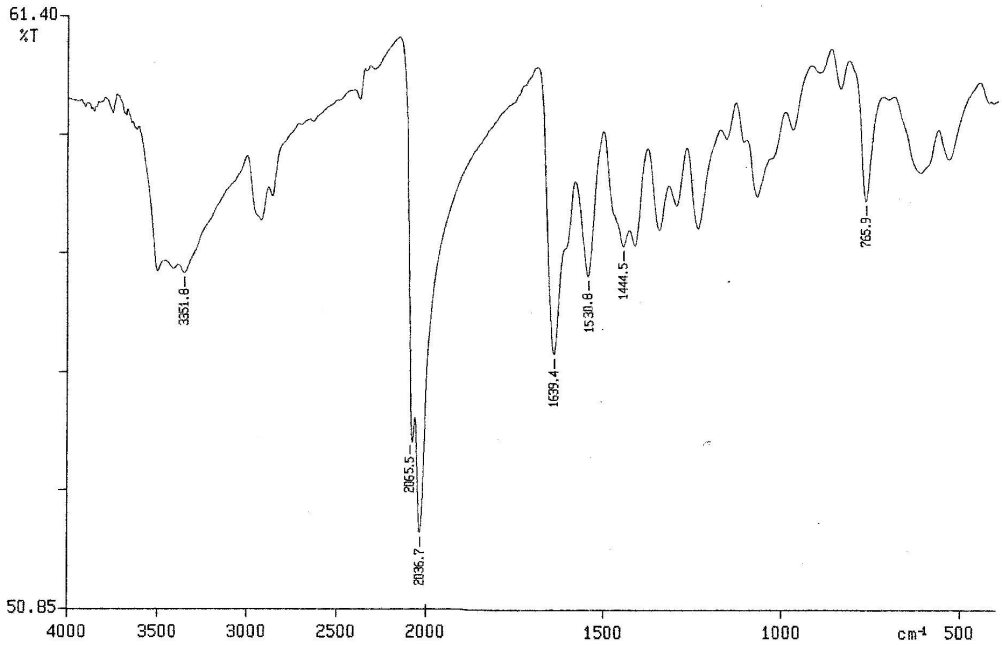

Figure. S4. FT-IR spectrum of complex **4.**

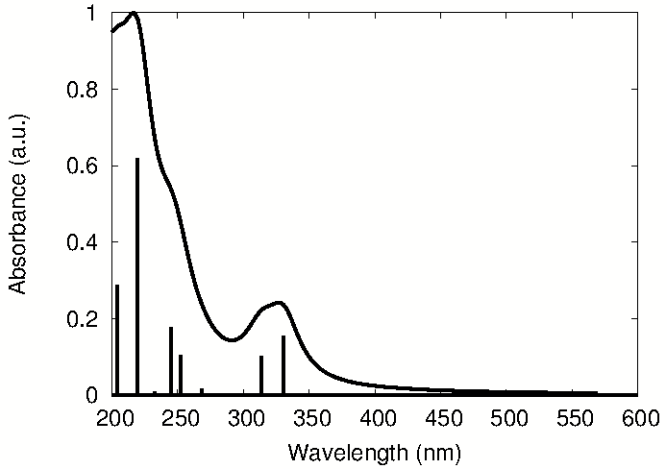

Figure. S4. Computed PCM-TDDFT UV-Vis absorption spectrum of HL^1. The theoretical spectrum is convoluted with a Lorentzian function with a full width at half-maximum (fwhm) of 15 nm; the corresponding transitions are marked with vertical lines.

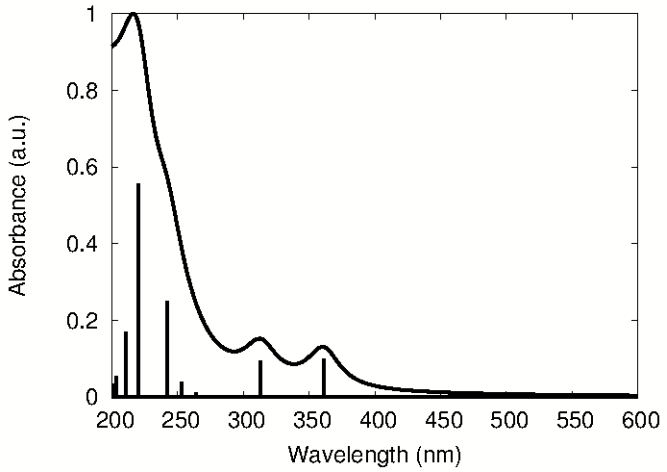

Figure. S5. Computed PCM-TDDFT UV-Vis absorption spectrum of HL^2. The theoretical spectrum is convoluted with a Lorentzian function with a full width at half-maximum (fwhm) of 15 nm; the corresponding transitions are marked with vertical lines.

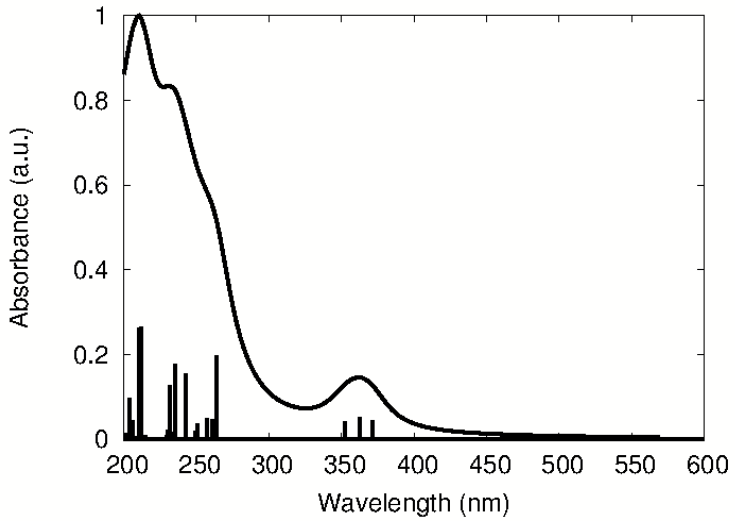

Figure. S6. Computed PCM-TDDFT UV-Vis absorption spectrum of the complex cation of complex **1**. The theoretical spectrum is convoluted with a Lorentzian function with a full width at half-maximum (fwhm) of 15 nm; the corresponding transitions are marked with vertical lines.

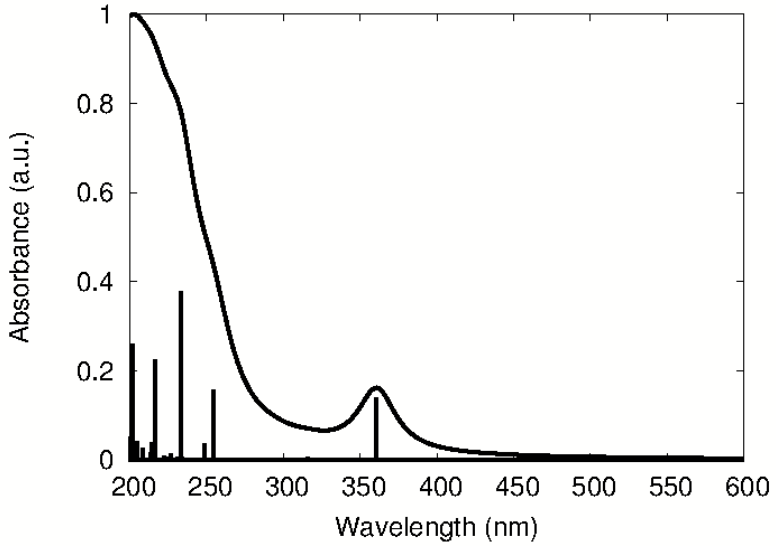

Figure. S7. Computed PCM-TDDFT UV-Vis absorption spectrum of the anionic complex of complex **2**. The theoretical spectrum is convoluted with a Lorentzian function with a full width at half-maximum (fwhm) of 15 nm; the corresponding transitions are marked with vertical lines.

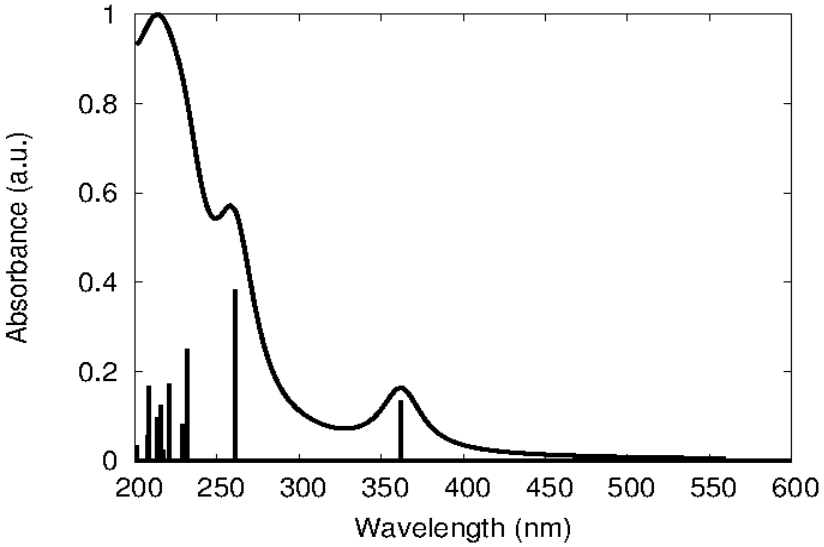

Figure. S8. Computed PCM-TDDFT UV-Vis absorption spectrum of the cationic complex of complex **2**. The theoretical spectrum is convoluted with a Lorentzian function with a full width at half-maximum (fwhm) of 15 nm; the corresponding transitions are marked with vertical lines.

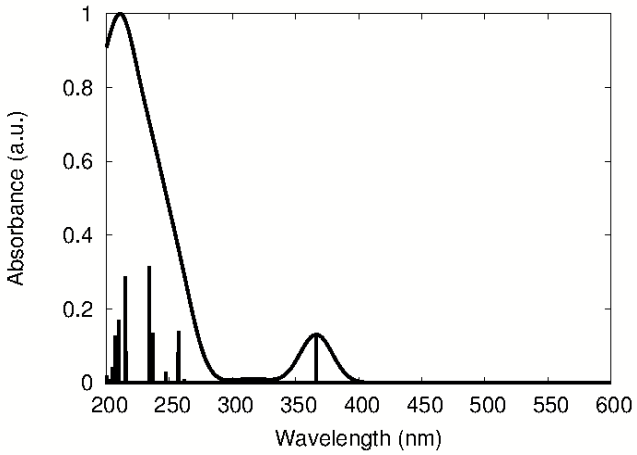

Figure. S9. Computed PCM-TDDFT UV-Vis absorption spectrum of the independent unito of polymeric complex **3**. The theoretical spectrum is convoluted with a Lorentzian function with a full width at half-maximum (fwhm) of 15 nm; the corresponding transitions are marked with vertical lines.

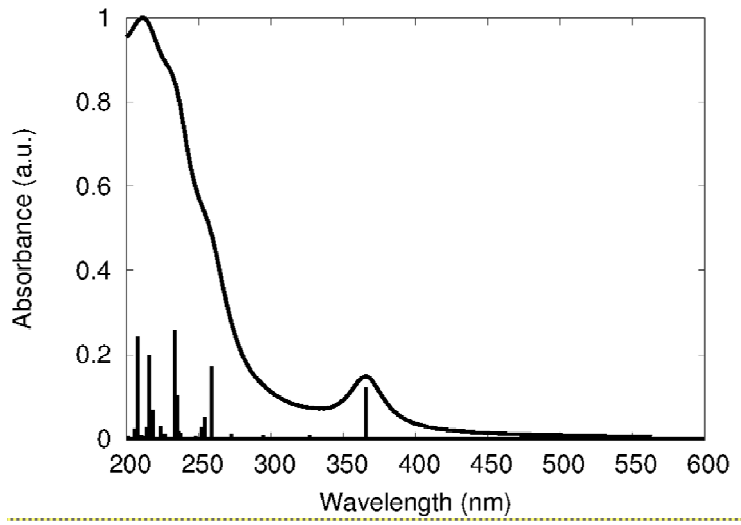

Figure S10. Computed PCM-TDDFT UV-Vis absorption spectrum of the independent unito of polymeric complex **4**. The theoretical spectrum is convoluted with a Lorentzian function with a full width at half-maximum (fwhm) of 15 nm; the corresponding transitions are marked with vertical lines.

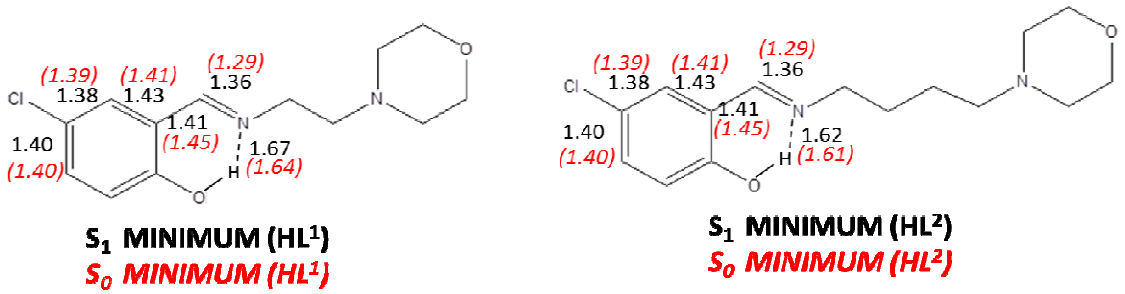

Figure. S11. Main bond distances (Å) of the lowest singlet excited state (S_1) and ground state (S_0) optimized geometries

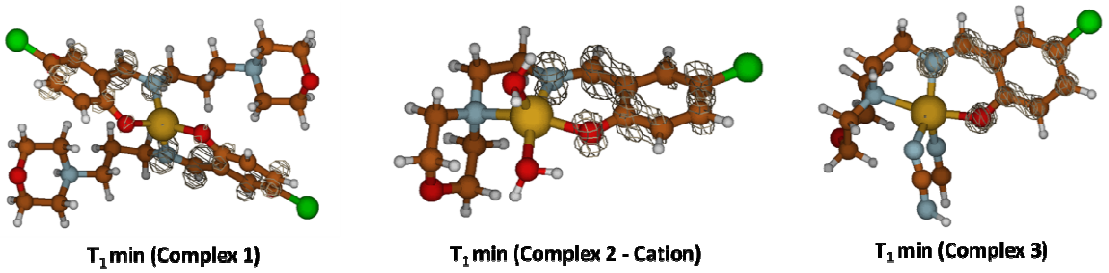

Figure. S12. Spin density distributions (B3LYP/6-31G*) plots at the lowest triplet (T_1) optimized minimum structures of complexes **1-3.**

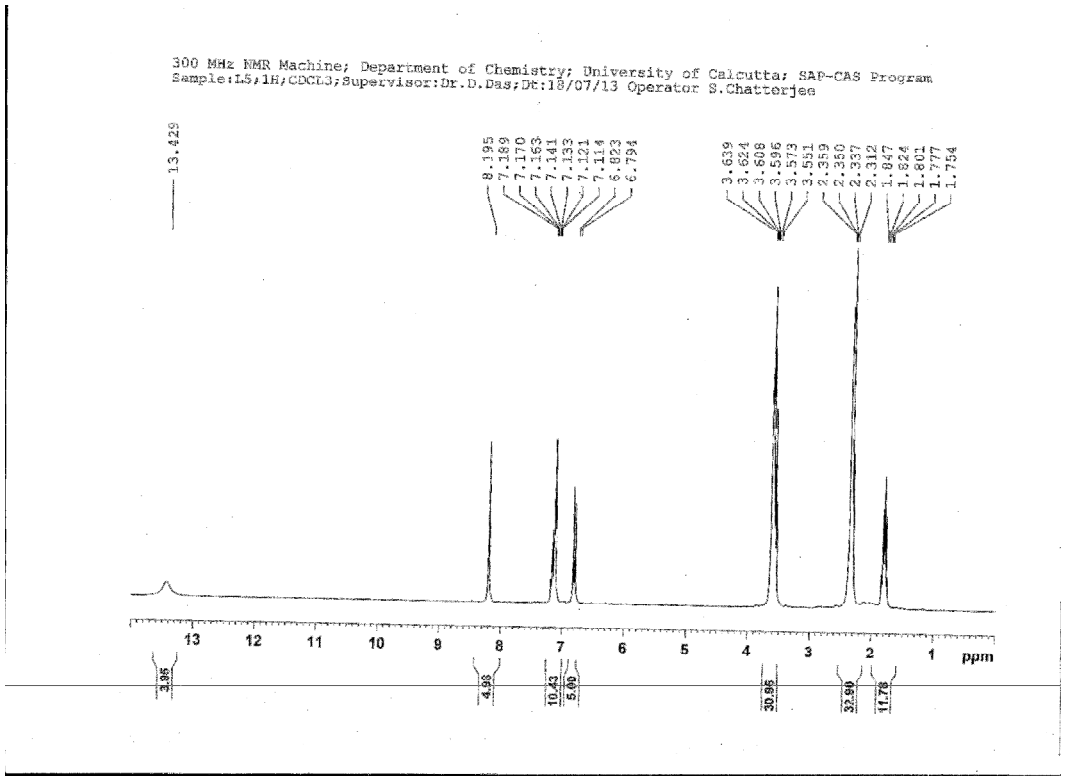

Figure. S13. ^{1}H NMR spectra of ligand HL^{2}.

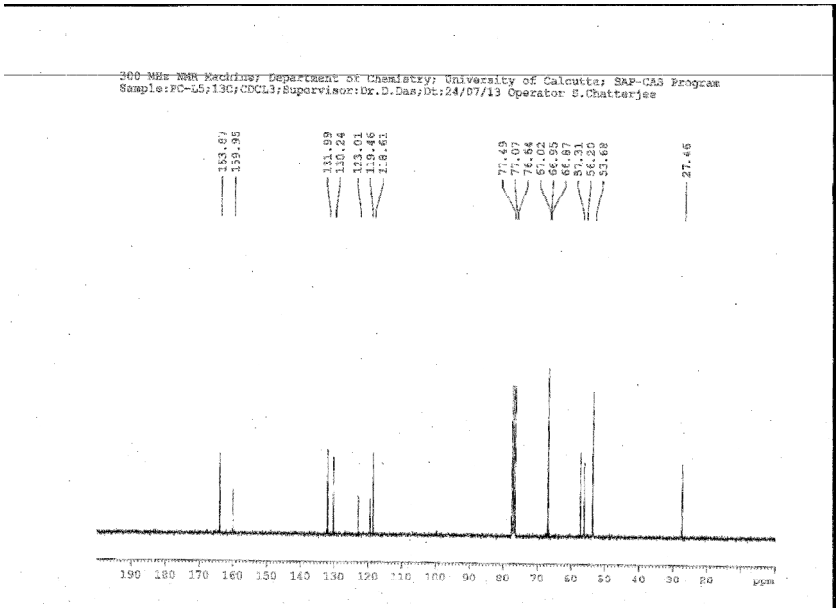

Figure. S14. ^{13}C NMR spectra of ligand HL^{2}.

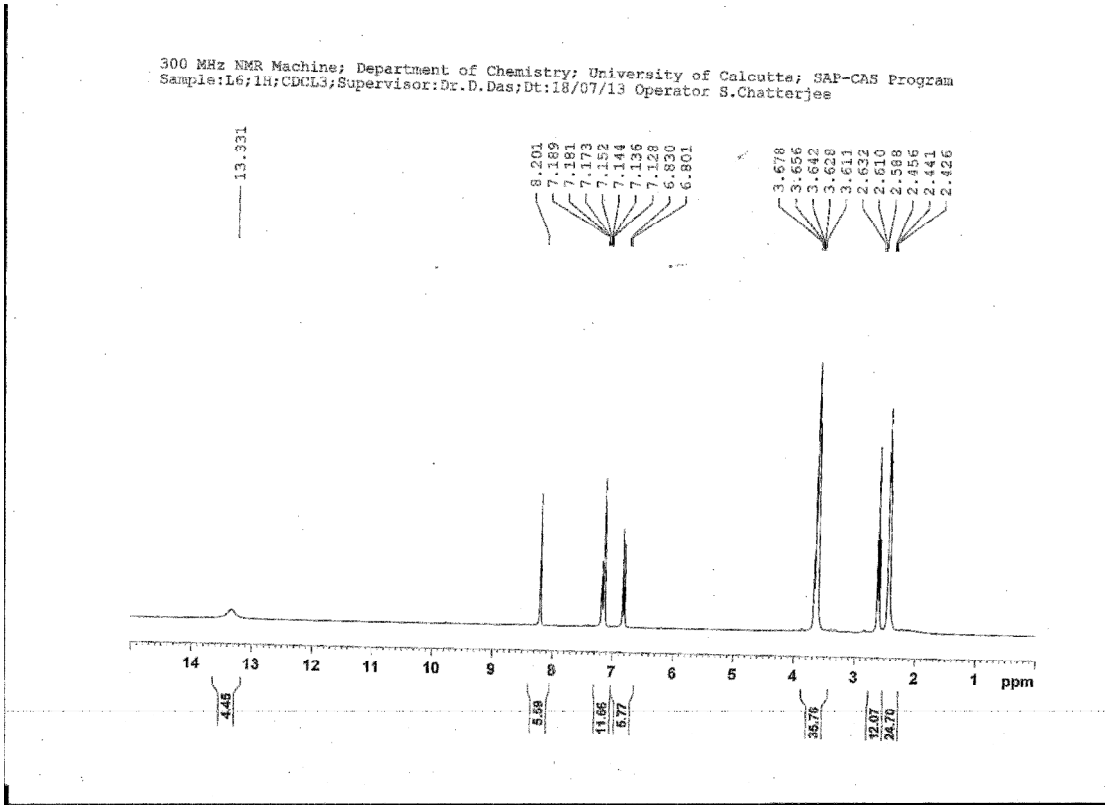

Figure. S15. ^{1}H NMR spectra of ligand HL[1].

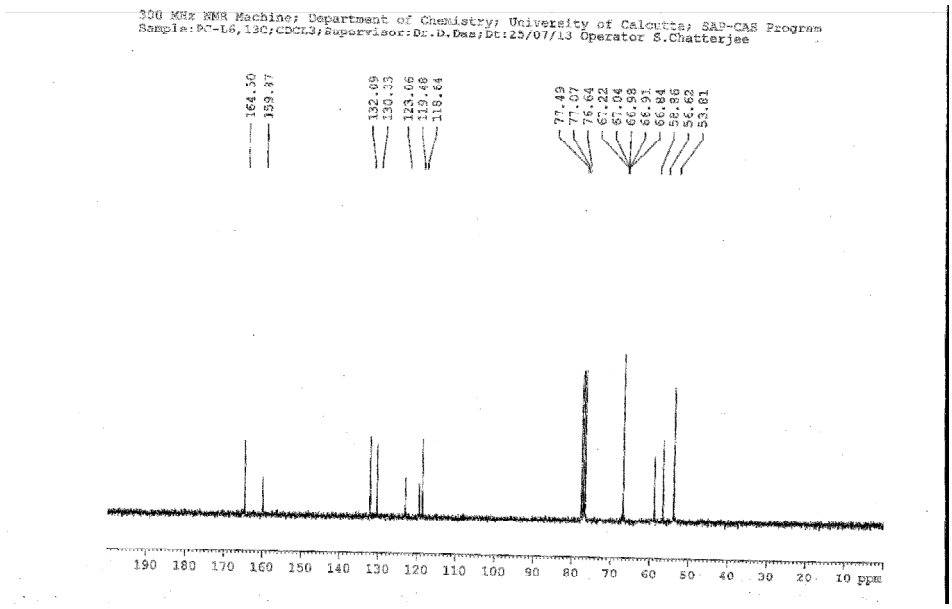

Figure. S16. ^{13}C NMR spectra of ligand HL[1].

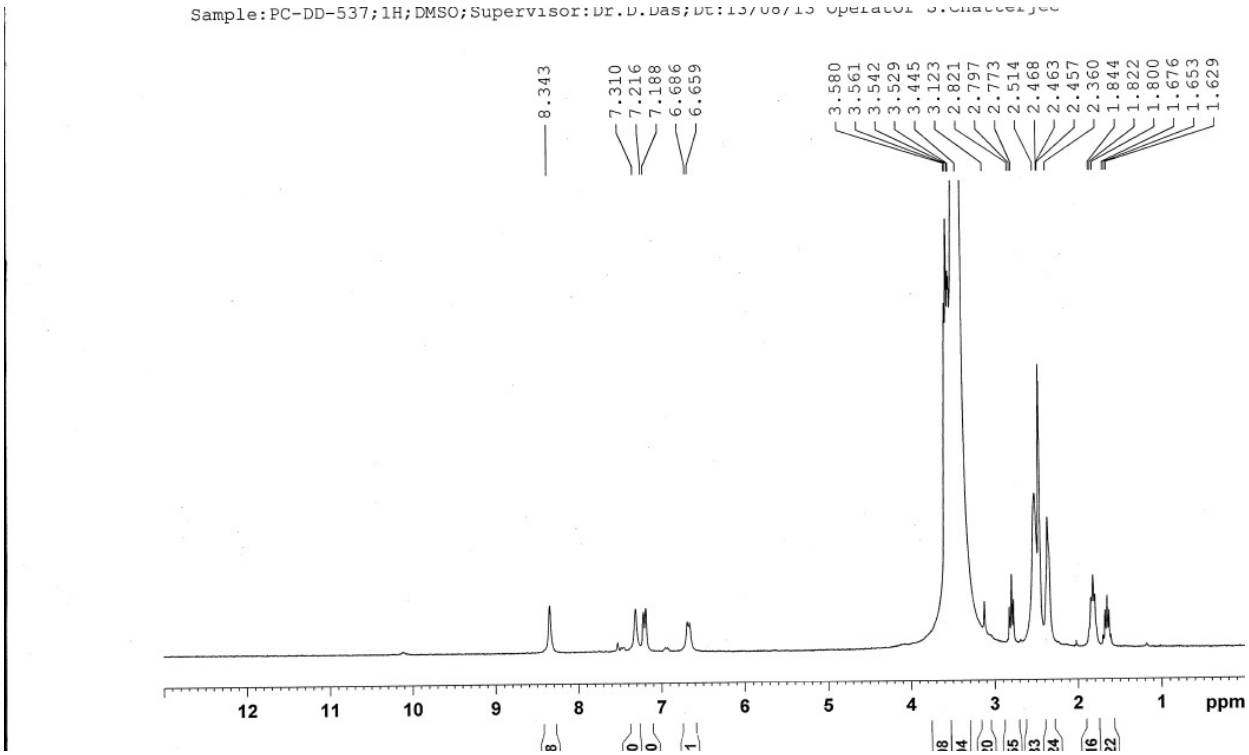

Figure. S17. ^{1}H NMR spectra of complex **1**.

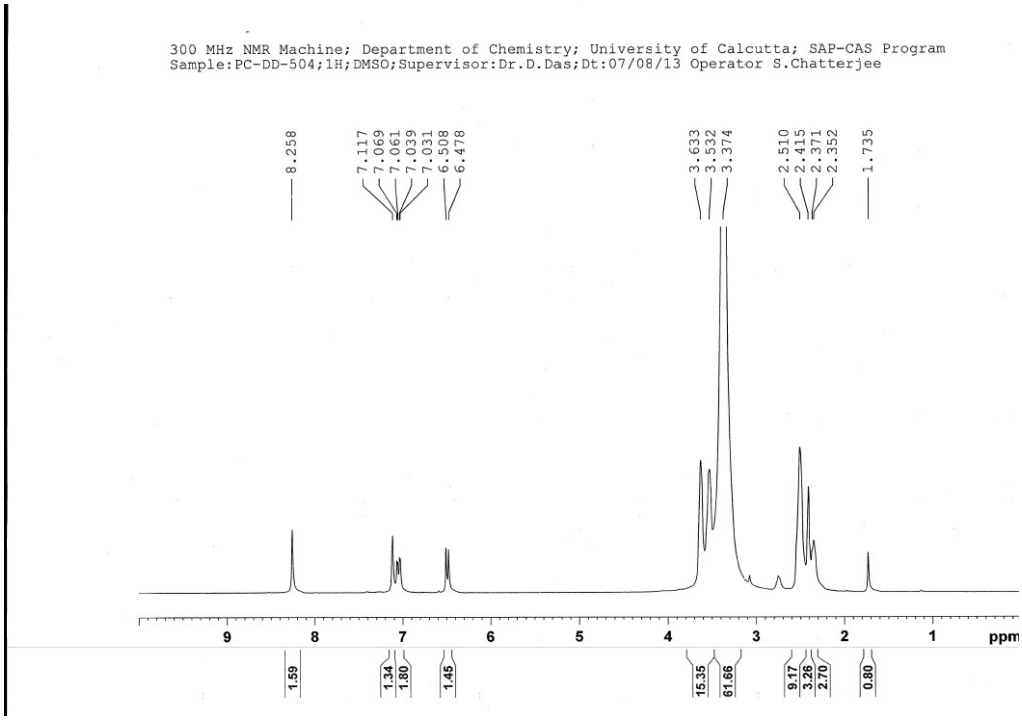

Figure. S18. ^{1}H NMR spectra of complex **2**.

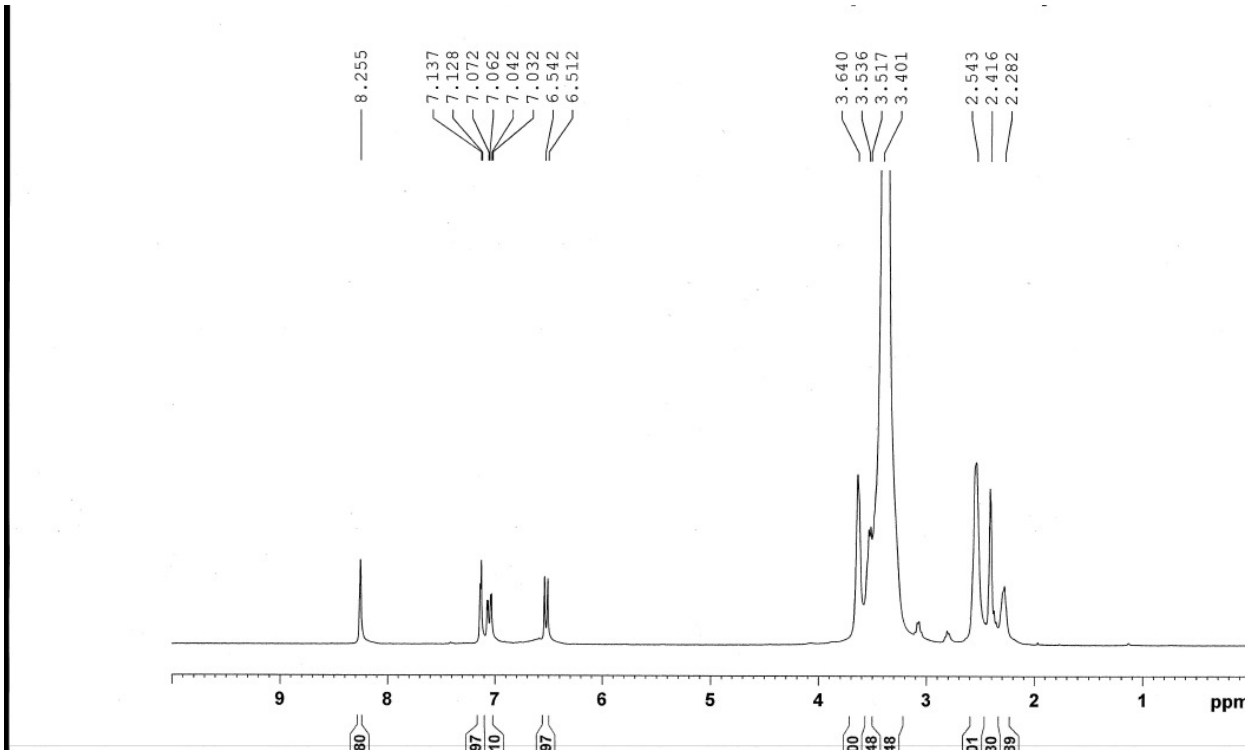

Figure. S19. ^{1}H NMR spectra of complex **3**.

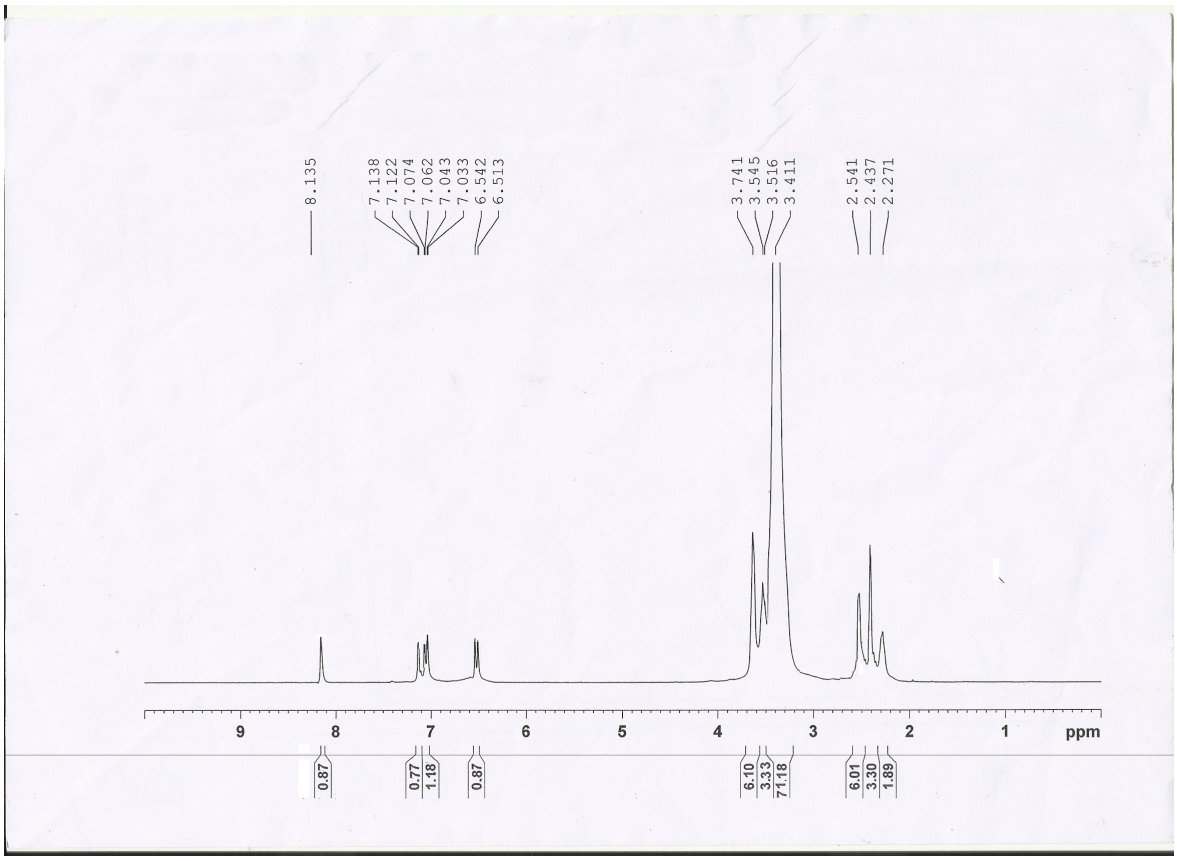

Figure. S20. ^{1}H NMR spectra of complex **4**.

Table-S1: Absorption data of two ligands and three complexes in methanol at 298K.

System	λ_{max}(nm) [ε($M^{-1}cm^{-1}$)]
HL^1	**251** (8970), **275** (3184), **325** (3338), **413** (1754)
HL^2	**251** (8619), **276** (2397), **325** (3196), **413** (1411)
Complex 1	**223** (23534), **268** (4118), **369** (2700)
Complex 2	**226** (17450), **268** (4074), **377** (2870)
Complex 3	**226** (7540), **270** (1780), **377** (1160)

Table - S2: Cartesian coordinates of all species

HL^1

C	1.205679	0.527181	0.215154
C	1.798475	-0.746373	0.280652
C	2.997920	-0.985316	-0.374231
C	3.631504	0.029164	-1.104313
C	3.056018	1.294210	-1.179152
C	1.843209	1.562857	-0.525646
H	1.306271	-1.535769	0.849392
O	1.294709	2.791967	-0.602715
H	4.573284	-0.173997	-1.611837
H	3.540016	2.090375	-1.743962
H	-3.572539	-2.774566	1.510815
C	-0.054114	0.775389	0.891685
N	-0.605857	1.944018	0.858342
C	-1.924891	2.083835	1.447097
H	-3.997400	1.910381	0.871412
C	-3.007570	1.651858	0.440666
N	-2.903757	0.242360	0.101967
C	-3.256769	-1.544410	-1.521125
C	-3.529815	-0.087412	-1.177045
C	-3.412869	-0.643412	1.147074
C	-3.144683	-2.092548	0.765822
O	-3.751297	-2.424659	-0.495056
H	-2.052594	-2.257861	0.700164
H	-2.167265	-1.695271	-1.636358
H	-3.766657	-1.826313	-2.450703
H	-4.629986	0.078628	-1.145344

H	-3.108012	0.557765	-1.961891
H	-4.505667	-0.495617	1.300226
H	-2.905899	-0.428307	2.099272
Cl	3.735469	-2.576988	-0.289626
H	0.411091	2.728759	-0.043551
H	-0.509442	-0.062151	1.440518
H	-2.097742	3.133764	1.712170
H	-2.012652	1.478383	2.363818
H	-2.882267	2.237487	-0.481644

HL^2

C	1.283921	0.502817	-0.133893
C	1.809421	-0.798504	-0.042106
C	2.963878	-1.128241	-0.737028
C	3.618089	-0.178201	-1.532812
C	3.108266	1.112721	-1.635320
C	1.940557	1.471859	-0.944465
H	1.301848	-1.536211	0.580115
O	1.452649	2.723898	-1.052153
H	4.524829	-0.451877	-2.070146
H	3.609035	1.858894	-2.251393
H	-4.911002	-1.720458	2.281163
C	0.073492	0.845548	0.589592
N	-0.429925	2.031499	0.519167
C	-1.684200	2.293056	1.210790
C	-2.842181	2.418881	0.210060
C	-2.975756	1.190868	-0.694273
N	-2.954470	-0.067705	0.048217
C	-2.711950	-2.495114	-0.034868
C	-2.821019	-1.213852	-0.847689
C	-4.130382	-0.243746	0.898468
C	-4.008401	-1.542299	1.683530
O	-3.863055	-2.675913	0.808937
H	-3.129415	-1.484057	2.352538
H	-1.802486	-2.454837	0.594365
H	-2.662239	-3.371503	-0.692916
H	-3.690628	-1.292286	-1.539238
H	-1.912597	-1.089012	-1.457395
H	-5.064937	-0.263703	0.291397
H	-4.203360	0.594111	1.607628
Cl	3.618132	-2.753519	-0.619245
H	0.593286	2.731954	-0.456587
H	-0.412971	0.056479	1.184046
H	-1.587460	3.235147	1.768253
H	-1.904492	1.481598	1.923937
H	-2.695265	3.302846	-0.427446
H	-3.764499	2.587440	0.784824
H	-2.122197	1.166570	-1.389205
H	-3.895832	1.285047	-1.312479

$[Zn(L^1H)_2](ClO_4)_2$

Zn	12.067855	8.791677	12.439224
Cl	12.737554	9.792442	5.370153
Cl	9.170707	6.438976	18.570172
O	13.024626	9.993916	11.267550
O	10.863346	3.035330	15.954819
O	12.673397	8.403822	14.238246
O	9.137933	12.135485	7.235834
N	11.960002	7.248891	11.145905
N	11.661429	4.330405	13.502256
H	11.366145	3.589600	12.850169
N	10.156595	9.220731	12.936652
N	9.131765	11.330495	10.004247
H	8.089908	11.270746	10.142840
C	12.968955	9.868520	9.955798
C	13.301040	11.000318	9.165491
H	13.599734	11.909385	9.687068
C	13.235564	10.980424	7.782410
H	13.480540	11.873337	7.208553
C	12.842600	9.806030	7.120201
C	12.529642	8.672023	7.842074
H	12.209040	7.765625	7.329503
C	12.574647	8.672891	9.258470
C	12.150461	7.441853	9.876930
H	11.933626	6.614705	9.188183
C	11.415849	5.970675	11.592854
H	11.332290	5.254039	10.763816
H	10.398971	6.168909	11.964065
C	12.307512	5.432852	12.710533
H	13.236130	5.020536	12.301100
H	12.561601	6.221646	13.429868
C	12.659849	3.720229	14.458469
H	13.516146	3.374074	13.870241
H	12.964348	4.529960	15.133903
C	12.000696	2.579949	15.215598
H	11.697538	1.786022	14.507931
H	12.717647	2.163829	15.931528
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H	9.546031	2.800134	14.354752
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H	9.696638	5.153585	13.588397
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C	11.839469	8.017651	15.181959
C	12.371161	7.319922	16.299039
H	13.448045	7.154641	16.323703
C	11.570100	6.842557	17.322940

H	12.010180	6.295339	18.155473
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C	9.619489	7.752422	16.229001
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C	10.416020	8.230452	15.158699
C	9.682263	8.860877	14.089047
H	8.608385	9.004824	14.276512
C	9.231807	9.721343	11.923581
H	8.230080	9.892619	12.346517
H	9.147507	8.942252	11.150653
C	9.787438	11.008232	11.313938
H	10.865650	10.928952	11.124323
H	9.603138	11.859660	11.977555
C	9.457506	12.737537	9.580321
H	10.548766	12.788609	9.469803
H	9.123577	13.408707	10.379758
C	8.748473	13.045243	8.270552
H	7.653296	12.999410	8.419493
H	9.020822	14.054219	7.941657
C	8.801132	10.796544	7.614803
H	9.118892	10.131441	6.803545
H	7.705663	10.706840	7.741742
C	9.511789	10.383376	8.893580
H	9.232722	9.360277	9.171348
H	10.601998	10.456343	8.778809
Cl	6.034401	11.803314	11.717446
O	5.879310	10.836410	12.825359
O	4.783941	12.560066	11.512063
O	7.159593	12.727798	12.004063
O	6.362297	11.049202	10.454389
Cl	8.933536	6.376075	8.521521
O	8.826425	6.998392	9.869126
O	9.374216	7.396847	7.539813
O	9.928212	5.272030	8.569292
O	7.609056	5.833722	8.123578

$[Zn(L^2H)_2](ClO_4)_2$

Zn	10.542926	7.733982	11.525050
Cl	14.009865	8.186483	5.174615
Cl	7.944126	8.521234	18.257055
O	11.711299	8.966431	10.561007
O	13.148567	3.858110	16.311017
O	11.163728	7.680461	13.374125
O	10.938164	13.879379	9.035930
N	10.698173	6.207134	10.252951
N	11.906781	3.822352	13.710896
H	11.320514	2.983222	13.827593
N	8.630917	8.148468	11.928143

N	9.046053	11.827244	9.748419
H	8.345270	11.985730	9.010507
C	12.215098	8.718099	9.373524
C	13.018385	9.719030	8.759900
H	13.206978	10.631808	9.324630
C	13.559275	9.564123	7.495550
H	14.165381	10.355543	7.055933
C	13.328001	8.377271	6.780669
C	12.581185	7.361857	7.342782
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C	12.015639	7.498356	8.635627
C	11.303347	6.340798	9.112221
H	11.282866	5.487359	8.421340
C	10.020447	4.938092	10.542568
H	10.391600	4.147899	9.873573
H	8.946845	5.065246	10.345703
C	10.213268	4.546498	12.005450
H	9.785062	5.332940	12.645919
H	9.653557	3.619417	12.195509
C	11.687517	4.344478	12.318151
H	12.135697	3.607323	11.640240
H	12.253615	5.282542	12.251472
C	13.341414	3.408745	13.922415
H	13.580132	2.647993	13.171803
H	13.946977	4.307794	13.756532
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C	11.773229	4.218607	16.148998
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H	11.131273	3.331593	16.304351
C	11.511598	4.813359	14.775831
H	10.450122	5.051689	14.649717
H	12.110966	5.711665	14.587271
C	10.393484	7.894402	14.416645
C	10.988906	7.871890	15.708300
H	12.065360	7.710761	15.765516
C	10.254676	8.055188	16.866909
H	10.746645	8.029348	17.838659
C	8.871075	8.284781	16.785528
C	8.246888	8.338859	15.556045
H	7.177720	8.541852	15.488760
C	8.977414	8.146081	14.355841
C	8.202300	8.272496	13.147791
H	7.143890	8.527066	13.297839
C	7.692057	8.379697	10.824634
H	6.718314	8.709064	11.216156
H	7.557474	7.443107	10.265794
C	8.267450	9.429408	9.869884
H	9.182660	9.026051	9.412114
H	7.541441	9.602818	9.062660

C	8.551458	10.715123	10.629634
H	9.333420	10.569711	11.386765
H	7.645669	11.092110	11.122326
C	9.181537	13.107109	10.536231
H	9.904777	12.896376	11.333569
H	8.201122	13.333358	10.971186
C	9.673606	14.214962	9.620674
H	8.931256	14.404374	8.823635
H	9.812411	15.131541	10.204108
C	10.803180	12.696659	8.241342
H	11.784273	12.478300	7.803275
H	10.079129	12.873732	7.424805
C	10.357504	11.509096	9.077562
H	10.217740	10.622848	8.449616
H	11.060629	11.274212	9.885711
Cl	5.446170	11.472706	12.992564
O	5.839931	10.519767	14.062068
O	4.176704	12.146704	13.366165
O	6.516502	12.490989	12.816239
O	5.261202	10.732477	11.716274
Cl	7.784996	5.731670	7.593050
O	7.045571	5.433546	8.850942
O	8.283437	7.126291	7.634609
O	8.929499	4.793935	7.459865
O	6.867528	5.560570	6.434028

$[Zn(L^1)(H_2O)_2][Zn(L^1)(SCN)_2]$

Zn	1.680916	1.583092	12.329774
S	3.724944	3.458657	8.685053
S	-2.860999	1.472366	11.125931
Cl	7.614678	-2.857539	11.851026
O	2.514479	0.019442	11.088619
O	-0.081511	5.469740	13.232878
N	2.758242	0.769722	13.855832
N	0.864559	2.856170	14.059513
N	2.731658	2.936574	11.274659
N	-0.089839	1.231824	11.525435
C	3.652133	-0.595053	11.282923
C	4.289244	-1.284340	10.214356
H	3.814222	-1.283039	9.235593
C	5.484476	-1.961406	10.381849
H	5.946141	-2.474200	9.538233
C	6.099520	-1.991697	11.645168
C	5.515111	-1.350665	12.719296
H	5.987069	-1.378304	13.702107
C	4.299316	-0.638645	12.566194

C	3.793921	-0.005103	13.754181
H	4.374799	-0.209276	14.666299
C	2.464116	1.333237	15.179891
H	3.194414	2.124822	15.403725
H	2.551864	0.567241	15.961875
C	1.055817	1.901677	15.177547
H	0.331188	1.087036	15.034541
H	0.843843	2.390742	16.143764
C	-0.572602	3.211810	13.982236
H	-0.903400	3.601979	14.963209
H	-1.147898	2.305312	13.754993
C	-0.808196	4.271555	12.920558
H	-0.490096	3.895306	11.932407
H	-1.871761	4.536771	12.882283
C	1.321139	5.163452	13.256074
H	1.850198	6.090949	13.507429
H	1.637759	4.821780	12.257162
C	1.648198	4.097756	14.293636
H	2.720746	3.866591	14.240229
H	1.418780	4.480679	15.306487
C	3.148446	3.155835	10.193108
C	-1.262846	1.329097	11.356188
Zn	1.836693	2.308981	7.555781
Cl	-1.967517	8.501125	8.388347
N	1.598573	3.748344	6.095722
N	2.728888	1.183299	5.858835
O	0.007477	2.936444	8.278576
O	4.191407	-1.123999	6.842497
O	1.360120	0.786008	8.913754
H	1.950306	0.454130	9.682132
H	0.605206	1.198736	9.388606
O	-0.971127	1.118279	6.463868
H	-1.114248	1.607640	5.636220
H	-0.747086	1.823483	7.124184
C	-0.396963	4.187114	8.268330
C	-1.330677	4.618589	9.246314
H	-1.675645	3.881334	9.972076
C	-1.798567	5.921687	9.290685
H	-2.505214	6.227439	10.062110
C	-1.364297	6.850793	8.330609
C	-0.478582	6.472293	7.339190
H	-0.155790	7.188596	6.582878
C	0.028601	5.152701	7.291667
C	0.922596	4.843283	6.201782
H	1.012998	5.608433	5.415348
C	2.430363	3.476929	4.935144
H	3.472306	3.750783	5.164457
H	2.115167	4.048891	4.051545
C	2.328060	1.979832	4.662989
H	1.282042	1.727896	4.442862
H	2.949152	1.692832	3.800026

C	4.214207	1.150368	5.969968
H	4.587550	2.163412	6.170166
H	4.638250	0.800236	5.011446
C	4.639427	0.216108	7.088008
H	5.733434	0.183411	7.153065
H	4.236972	0.578650	8.052666
C	2.756012	-1.143867	6.752003
H	2.318072	-0.863403	7.722239
H	2.466130	-2.174336	6.514916
C	2.241857	-0.212968	5.667246
H	2.587203	-0.571203	4.680843
H	1.143206	-0.192436	5.681432

$[Zn(L^2)(H_2O)_2][Zn(L^2)(SCN)_2]$

Zn	2.203668	1.466388	7.330643
Cl	-2.712406	5.908773	10.134693
N	1.864508	3.258589	6.577023
N	4.133745	1.009370	6.824622
O	0.944319	1.476313	8.777504
O	4.678776	-1.550407	8.072576
O	-0.361701	-0.762459	8.204139
C	1.006667	4.050524	7.137691
C	4.639071	-0.335301	8.833395
O	0.998927	0.171078	6.141761
C	2.673278	3.740350	5.446371
C	5.055894	0.854736	7.994938
C	0.173037	2.526378	9.029273
C	-0.726965	2.413867	10.114877
C	3.807223	-1.441931	6.947311
C	-1.607088	3.430070	10.444324
C	4.625210	2.159474	5.983459
C	-1.599245	4.622577	9.705306
C	-0.724035	4.784356	8.650979
C	4.193619	-0.270691	6.051796
C	0.172382	3.750547	8.277693
H	0.031661	0.043728	8.650173
H	5.324823	-0.462911	9.679555
H	3.616256	-0.180204	9.234234
H	0.395652	-0.314770	6.794437
H	3.264244	4.607521	5.779941
H	2.011706	4.074761	4.634408
H	5.009900	1.777681	8.588546
H	6.078139	0.714283	7.606338
H	-0.683543	1.498056	10.705767
H	2.764100	-1.324229	7.304483
H	3.881984	-2.378965	6.383184
H	-2.299179	3.309384	11.278297
H	5.563482	1.835715	5.507552

H	4.861143	2.972438	6.685089
H	-0.719449	5.712848	8.080077
H	5.226870	-0.404287	5.690590
H	3.530714	-0.205695	5.178809
H	0.880500	5.060302	6.720577
H	-1.314797	-0.579479	8.132531
H	1.426580	-0.514630	5.601254
C	3.616604	2.650271	4.936124
H	4.174793	3.062438	4.085978
H	3.032099	1.804816	4.539164
Zn	1.229716	2.059842	12.975431
S	3.821123	3.969668	9.456446
S	-3.431871	2.502946	13.909024
Cl	5.265589	-3.612789	10.967272
O	0.868656	0.170242	12.051983
O	0.131083	6.334329	12.493408
N	2.464856	1.074712	14.290954
N	1.568104	4.260415	13.951136
N	2.372717	2.614152	11.453404
N	-0.679677	2.104594	13.483129
C	1.856067	-0.633267	11.835236
C	1.790143	-1.588063	10.769675
C	-1.837737	2.259923	13.670154
C	2.810828	-2.481861	10.508704
C	2.228311	5.238546	13.053090
C	3.964429	-2.480193	11.314768
C	4.075261	-1.604615	12.374157
C	0.318921	4.886449	14.453689
C	3.046635	-0.671195	12.658449
C	3.205944	0.092966	13.864528
C	1.296321	5.696762	11.944158
C	2.745917	1.540026	15.661445
C	2.984324	3.170202	10.609210
C	-0.559072	5.379481	13.312249
C	2.486532	4.008739	15.089722
H	0.896007	-1.582073	10.146780
H	2.735854	-3.180447	9.676245
H	3.127243	4.775211	12.628809
H	2.535582	6.121840	13.648310
H	4.956866	-1.627251	13.016737
H	0.586458	5.745938	15.101255
H	-0.241490	4.158412	15.052955
H	4.039217	-0.234089	14.507777
H	1.803362	6.437177	11.312850
H	0.988513	4.838234	11.322068
H	3.834795	1.656757	15.793323
H	2.410557	0.764934	16.367139
H	-0.877277	4.529511	12.687476
H	-1.445617	5.882020	13.719684
C	2.046682	2.850095	15.989580
H	2.269524	3.092385	17.037169

H	0.957447	2.710065	15.924070
H	2.583481	4.943513	15.674605
H	3.477311	3.789467	14.661837

$[Zn(L^1)(H_2O)_2]^{1+}$

Zn	1.026563	-0.339310	-0.074965
Cl	-6.294208	0.404049	-0.143506
N	0.006443	1.380178	-0.116989
N	2.783977	0.962674	-0.218140
O	-0.685169	-1.440422	-0.120617
O	5.183164	-0.315737	0.793229
O	1.355574	-1.578678	1.614414
C	-1.283752	1.503564	-0.155621
C	4.183411	0.183416	1.693240
O	1.510604	-1.480950	-1.813468
C	0.870627	2.557229	-0.151375
C	3.397458	1.337687	1.090214
C	-1.907455	-0.971975	-0.119076
C	-2.991462	-1.894282	-0.102542
C	4.574710	-0.716383	-0.438953
C	-4.311654	-1.482842	-0.107526
C	2.168465	2.166822	-0.851830
C	-4.614586	-0.109766	-0.133565
C	-3.602533	0.827256	-0.151325
C	3.866252	0.451502	-1.101192
C	-2.241160	0.430443	-0.139534
H	0.535638	-2.113810	1.548057
H	4.706804	0.533690	2.590319
H	3.507253	-0.636925	1.984238
H	0.763716	-2.110185	-1.869713
H	1.077773	2.878939	0.880125
H	0.398280	3.395204	-0.681124
H	2.607975	1.645557	1.787751
H	4.073757	2.193870	0.919623
H	-2.746782	-2.956379	-0.084224
H	3.856520	-1.539961	-0.242952
H	5.372601	-1.093680	-1.088389
H	-5.116782	-2.216779	-0.092261
H	1.955024	1.905192	-1.897427
H	2.883799	3.003570	-0.836343
H	-3.837062	1.891842	-0.171336
H	4.594295	1.260582	-1.285395
H	3.427151	0.151817	-2.061177
H	-1.707072	2.517206	-0.207613
H	2.089125	-2.220153	1.597887
H	2.314879	-2.031214	-1.802075

$[Zn(L^2)(H_2O)_2]^{1+}$

Zn	1.088188	-0.245671	0.082955
Cl	-5.942853	-1.145104	-1.340785
N	0.331985	-0.123252	-1.734512
N	2.550953	1.205980	-0.154273
O	-0.594402	-0.383212	1.054687
O	2.010501	2.830953	2.178533
O	0.369245	-2.007672	2.926356
C	-0.934504	-0.265015	-1.964853
C	1.102447	2.800699	1.069317
O	2.011617	-1.865821	0.909541
C	1.260014	0.187660	-2.835343
C	1.826810	2.515951	-0.237206
C	-1.764947	-0.544667	0.446114
C	-2.899762	-0.770224	1.260310
C	2.711769	1.586744	2.275732
C	-4.163863	-0.956664	0.726069
C	3.319497	0.952615	-1.435329
C	-4.341436	-0.913382	-0.665156
C	-3.264479	-0.685762	-1.498630
C	3.488334	1.284186	1.005257
C	-1.960019	-0.501842	-0.976120
H	-0.215949	-1.418781	2.367541
H	0.619423	3.782952	1.018328
H	0.322711	2.034052	1.253711
H	1.500342	-2.068219	1.770536
H	1.130460	1.244618	-3.116677
H	1.012747	-0.425921	-3.712843
H	1.108441	2.471372	-1.067025
H	2.563539	3.308977	-0.443753
H	-2.754347	-0.794141	2.340455
H	1.988017	0.768835	2.479269
H	3.396557	1.663666	3.127645
H	-5.016265	-1.132710	1.380752
H	4.316833	0.594500	-1.151221
H	3.447890	1.919242	-1.944220
H	-3.403879	-0.646496	-2.578764
H	4.229282	2.076695	0.813522
H	4.015420	0.325182	1.099082
H	-1.286787	-0.196416	-3.003701
H	-0.089055	-2.864601	2.980671
H	2.951574	-1.782090	1.148752
C	2.700570	-0.070074	-2.393875
H	3.343739	-0.084558	-3.283832
H	2.758486	-1.081505	-1.955814

$[Zn(L^1)(SCN)_2]^{1-}$

Zn	-0.483636	0.082388	-0.241905
S	-1.775082	4.555054	-0.921943
S	-2.628185	-3.983147	-1.404494
Cl	6.830279	-0.850306	0.472384
O	1.263800	-0.107598	-1.355095
O	-4.973302	0.484383	0.600534
N	0.616777	0.247659	1.458850
N	-2.273184	0.005060	1.546692
N	-1.037966	1.838586	-0.955281
N	-1.283967	-1.538658	-1.028717
C	2.469198	-0.264682	-0.905992
C	3.536047	-0.526932	-1.823265
C	-1.842104	-2.572573	-1.185303
C	4.843005	-0.705749	-1.410872
C	-2.957721	1.304681	1.720969
C	5.162613	-0.625089	-0.042241
C	4.178121	-0.367523	0.888530
C	-3.290934	-1.061062	1.445927
C	2.828869	-0.186828	0.491437
C	1.901597	0.087657	1.553577
C	-3.992229	1.535119	0.628335
C	-0.131761	0.545899	2.678441
C	-1.336698	2.986794	-0.935251
C	-4.300131	-0.762131	0.351388
C	-1.405572	-0.284237	2.704175
H	3.282740	-0.587840	-2.882059
H	5.628297	-0.908321	-2.138862
H	-2.218610	2.117216	1.685997
H	-3.460357	1.329016	2.709911
H	4.426418	-0.299282	1.948614
H	-3.827492	-1.155233	2.411979
H	-2.784613	-2.012959	1.235762
H	2.354339	0.171152	2.553861
H	-4.530007	2.471794	0.820013
H	-3.494203	1.591187	-0.353633
H	-0.382220	1.617728	2.682910
H	0.467341	0.337502	3.577075
H	-3.790027	-0.715716	-0.626719
H	-5.069070	-1.543861	0.326455
H	-1.135389	-1.349343	2.659913
H	-1.946916	-0.107957	3.653121

$[Zn(L^2)(SCN)_2]^{1-}$

Zn	-0.586674	0.260483	0.239482

S	0.584564	-4.076957	-1.374926
S	-3.656135	2.508974	3.022551
Cl	6.558237	-0.316498	-0.707989
O	1.132185	0.271090	1.547779
O	-4.466079	-1.789306	-0.356049
N	0.459743	1.588863	-0.921714
N	-2.470033	0.135487	-1.266076
N	-0.126881	-1.626041	-0.182766
N	-1.690392	0.995300	1.694281
C	2.305891	0.142514	1.019336
C	3.362618	-0.499814	1.740043
C	-2.511970	1.640700	2.255660
C	4.634322	-0.646884	1.217889
C	-2.660454	-1.197336	-1.890673
C	4.930881	-0.135489	-0.060452
C	3.961390	0.516488	-0.793746
C	-3.760708	0.528472	-0.645834
C	2.644617	0.658589	-0.289359
C	1.741781	1.435630	-1.090215
C	-3.206377	-2.215853	-0.902476
C	-0.178290	2.609658	-1.772103
C	0.187228	-2.650899	-0.684652
C	-4.265221	-0.534816	0.316124
C	-2.138704	1.094983	-2.351059
H	3.130043	-0.887561	2.732410
H	5.411635	-1.152224	1.791035
H	-1.695795	-1.539896	-2.286587
H	-3.373123	-1.099397	-2.733174
H	4.198365	0.935073	-1.773009
H	-4.512424	0.672561	-1.447555
H	-3.641437	1.477646	-0.109327
H	2.216524	1.984356	-1.919678
H	-3.384024	-3.169161	-1.415779
H	-2.486578	-2.370253	-0.081748
H	0.243378	2.555344	-2.789779
H	0.071731	3.601040	-1.364509
H	-3.545261	-0.671838	1.141261
H	-5.235743	-0.230589	0.727102
C	-1.690582	2.463374	-1.831698
H	-2.076576	3.254844	-2.487616
H	-2.115605	2.649070	-0.834121
H	-3.020679	1.194143	-3.011833
H	-1.333120	0.641600	-2.949115

$[Zn(L^1H)_2]^{2+}$

Zn	-0.053523	0.014546	-0.374721

Cl	-6.846765	-0.886988	1.898655
Cl	6.780147	0.882477	1.782988
O	-1.083978	-1.288589	0.666491
O	0.696873	5.784630	0.613243
O	0.993813	1.299601	0.671084
O	-0.825779	-5.764928	0.509414
N	-1.579625	0.978118	-1.179068
N	0.235465	3.402535	-0.929113
H	0.469337	2.677557	-0.191037
N	1.455855	-0.935250	-1.223893
N	-0.369612	-3.357502	-0.994043
H	-0.591823	-2.644850	-0.240178
C	-2.378746	-1.130746	0.924155
C	-2.968358	-1.943541	1.918205
C	1.269596	-1.911420	-2.306832
C	-4.319205	-1.871452	2.217139
C	-0.894649	4.259112	-0.432311
C	-5.138754	-0.965426	1.525144
C	-4.600882	-0.133871	0.563955
C	0.761982	-4.225942	-0.522142
C	-3.218656	-0.186032	0.245999
C	-2.791926	0.756232	-0.752979
C	-1.924950	-4.938113	0.112520
C	-1.411351	1.972413	-2.248091
C	2.293638	1.138952	0.900040
C	2.902760	1.936733	1.894568
C	-0.061585	2.664590	-2.207393
C	-0.082188	-2.599147	-2.262376
C	4.259301	1.861228	2.165439
H	2.654972	5.626483	0.031805
C	-1.616809	-4.186706	-1.172325
C	5.065147	0.965781	1.444249
C	1.477651	4.239997	-1.104016
C	4.508497	0.148646	0.481489
C	0.330241	-4.954334	0.742522
C	1.794449	4.967919	0.192347
C	3.120427	0.205210	0.191054
C	2.675550	-0.720692	-0.815369
C	-0.454852	4.966804	0.841367
H	-0.236990	4.220120	1.627991
H	-2.322584	-2.627539	2.467164
H	2.089335	-2.642378	-2.307284
H	1.303254	-1.385304	-3.271493
H	-4.744890	-2.511102	2.988889
H	-1.756218	3.612146	-0.231015
H	-1.137307	4.972892	-1.229937
H	-5.234807	0.579442	0.037855
H	1.626704	-3.584421	-0.316981
H	0.995941	-4.926579	-1.333797
H	-3.597936	1.358957	-1.192288
H	-2.168251	-4.225296	0.920624

H	-2.787755	-5.591950	-0.054651
H	-2.233816	2.699985	-2.226773
H	-1.454845	1.462137	-3.220734
H	2.267731	2.611214	2.467293
H	-0.009738	3.391395	-3.025399
H	0.760842	1.946193	-2.332463
H	-0.144768	-3.311775	-3.092253
H	-0.903499	-1.876107	-2.366780
H	4.699971	2.489337	2.938276
H	3.473337	-1.317038	-1.277753
H	-1.262117	5.620911	1.187625
H	-1.421479	-4.876584	-2.002349
H	-2.432474	-3.504103	-1.442432
H	1.271959	4.944435	-1.919244
H	2.293216	3.565611	-1.393869
H	5.132130	-0.556403	-0.067546
H	1.138186	-5.616507	1.071329
H	0.121057	-4.220639	1.543646
H	2.045159	4.239926	0.984374

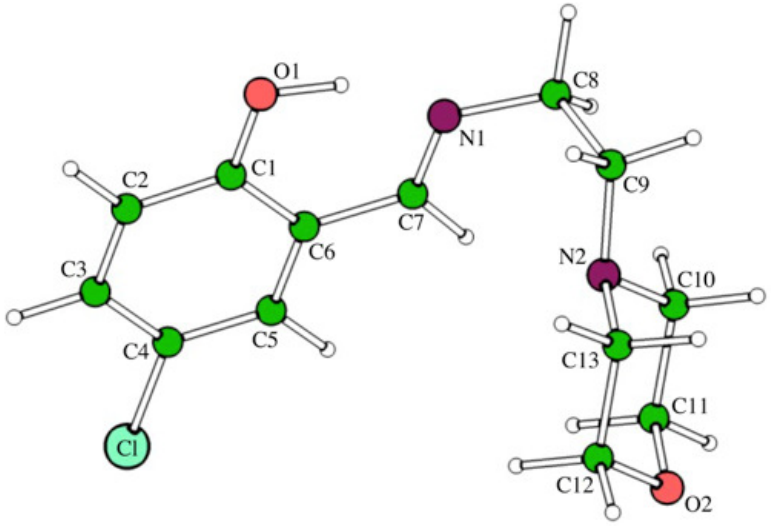
$[Zn(L^2H)_2]^{2+}$

Zn	-0.001078	0.050842	-0.092149
Cl	-5.781574	4.316329	0.931096
Cl	5.800871	-4.266767	0.505271
O	-1.557582	0.189877	1.071385
O	6.034047	2.616516	1.334287
O	1.574030	-0.174718	1.031526
O	-5.995106	-2.689168	1.309190
N	-0.373490	1.681574	-1.188797
N	3.799916	2.811734	-0.474677
H	4.324510	2.930824	-1.353297
N	0.344221	-1.503014	-1.302118
N	-3.793846	-2.717718	-0.547218
H	-4.337112	-2.781129	-1.420011
C	-2.445938	1.154418	1.002854
C	-3.514899	1.150172	1.940975
C	-0.564003	-1.772187	-2.422011
C	-4.520396	2.099965	1.922425
C	4.224371	1.502409	0.140361
C	-4.499912	3.118971	0.954531
C	-3.475106	3.180677	0.033392
C	-4.222591	-1.462349	0.168649
C	-2.433623	2.217068	0.031421
C	-1.426342	2.412936	-0.977471
C	-5.635933	-3.885382	0.607724
C	0.504637	2.027210	-2.312099
C	2.461340	-1.130113	0.875961
C	3.550337	-1.189391	1.788768

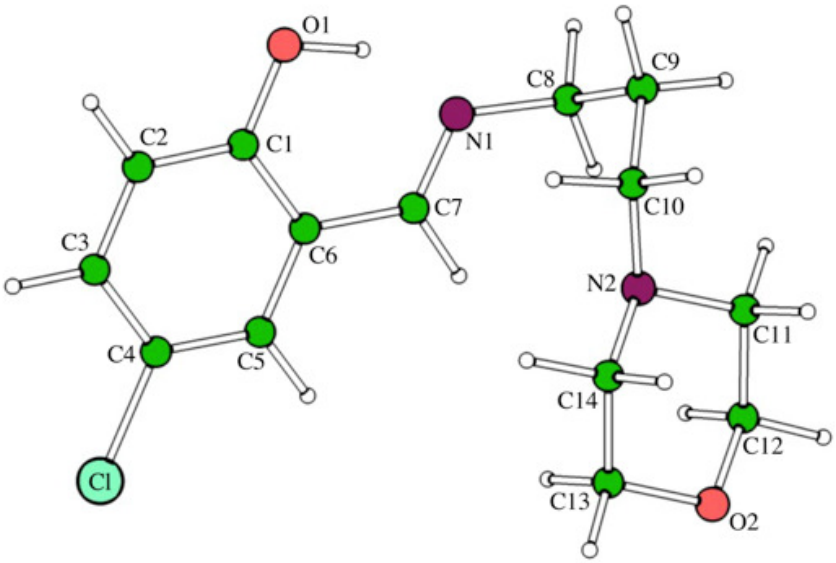
C	1.973683	1.884854	-1.921046
C	-2.021380	-1.671094	-1.976919
C	4.557347	-2.131499	1.680051
C	2.333663	2.852321	-0.804479
C	-4.148868	-3.917122	0.294909
C	4.517334	-3.078914	0.642628
C	4.190139	3.941948	0.444269
C	3.472225	-3.078877	-0.257480
C	-5.703532	-1.547194	0.498576
C	5.681489	3.865791	0.728601
C	2.429342	-2.121070	-0.167992
C	1.399815	-2.247869	-1.165395
C	5.712052	1.542595	0.445573
C	-2.336306	-2.712815	-0.914672
H	-3.522209	0.362099	2.693752
H	-0.353122	-2.760954	-2.857106
H	-0.387481	-1.016014	-3.200361
H	-5.325217	2.061791	2.655565
H	3.992790	0.697741	-0.565401
H	3.616798	1.383152	1.045279
H	-3.452808	3.977471	-0.710481
H	-4.016998	-0.605984	-0.482307
H	-3.597690	-1.397798	1.067377
H	-1.585486	3.281077	-1.632730
H	-6.217574	-3.959913	-0.329972
H	-5.888800	-4.734526	1.251502
H	0.289152	3.046726	-2.666428
H	0.298436	1.332748	-3.139411
H	3.573504	-0.455761	2.594462
H	2.590511	2.084229	-2.808587
H	2.160383	0.845014	-1.611375
H	-2.665152	-1.819439	-2.855296
H	-2.207097	-0.655749	-1.594319
H	5.378790	-2.141921	2.395378
H	2.111725	3.887150	-1.094931
H	1.803759	2.621874	0.128965
H	-3.540622	-3.844179	1.204172
H	-3.874877	-4.812588	-0.273188
H	3.595331	3.813137	1.356249
H	3.922010	4.880751	-0.052406
H	3.434786	-3.820949	-1.055301
H	-5.994673	-0.654927	1.065654
H	-6.295290	-1.586720	-0.435072
H	6.249287	3.999566	-0.210535
H	5.956925	4.661830	1.428615
H	1.542303	-3.069182	-1.882047
H	6.000301	0.606268	0.938315
H	6.286324	1.645732	-0.493865
H	-2.107645	-3.723244	-1.276717
H	-1.785198	-2.532726	0.01739

Computed NMR data of ligands and complexes at COSMO-KT2/ET-pVQZ, in ppm.

HL[1]



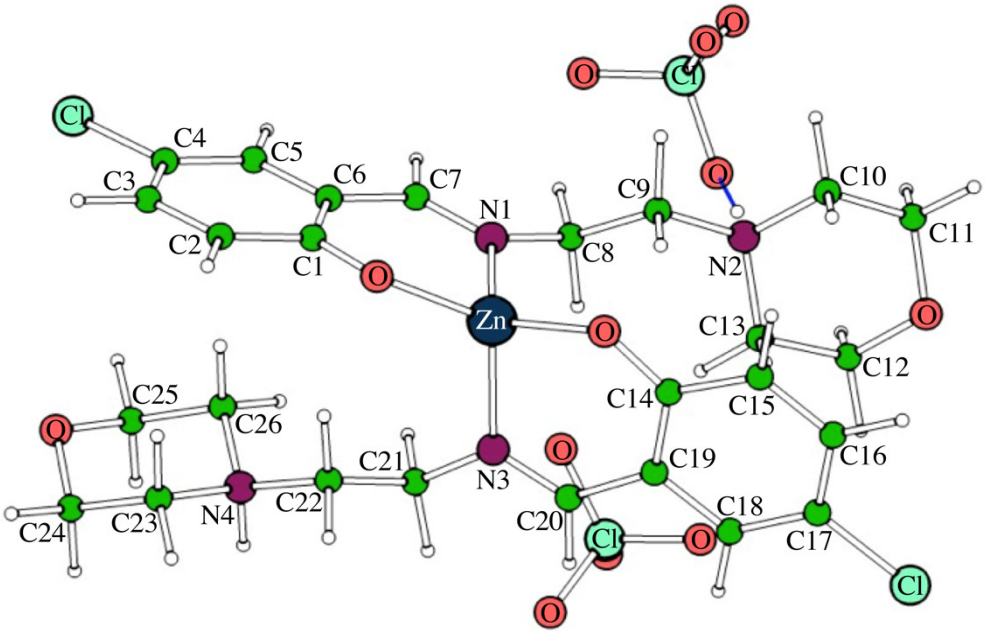
HL[2]



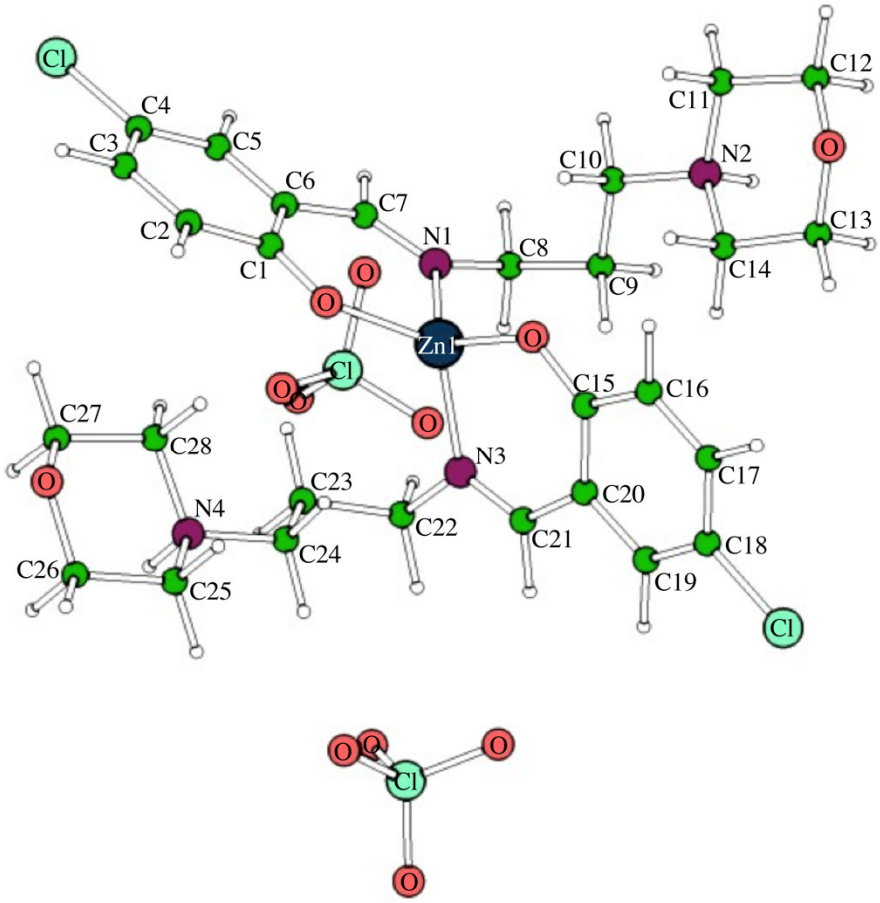
Computed NMR data at COSMO-KT2/ET-pVQZ, in ppm for two ligands.

HL[1]		HL[2]	
Atoms	^1H	Atoms	^1H
H(C2)	6.78	H(C2)	6.80
H(C3)	7.12	H(C3)	7.12
H(C5)	7.17	H(C5)	7.09
H(C7)	8.04	H(C7)	8.92
H(C8)	3.51, 3.69	H(C8)	3.58, 3.87
H(C9)	2.27, 2.52	H(C9)	1.63, 1.99
H(C10)	2.26, 2.50	H(C10)	2.04, 2.23
H(C11)	3.48, 3.76	H(C11)	1.79, 2.90
H(C12)	3.71, 3.92	H(C12)	3.84, 3.92
H(C13)	1.98, 3.15	H(C13)	3.82, 3.84
H(O1)	16.44	H(C14)	2.08, 2.17
		H(O1)	16.46

$[Zn(L^1H)_2](ClO_4)_2$



$[Zn(L^2H)_2](ClO_4)_2$

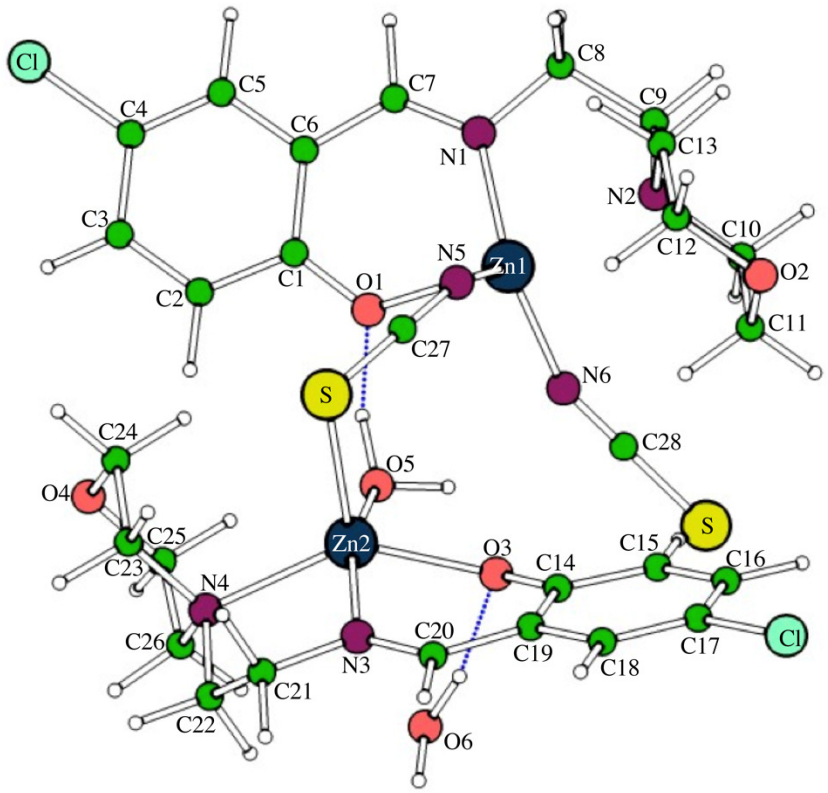


Computed NMR data for complex 1 along at COSMO-KT2/Et-pVQZ, in ppm.

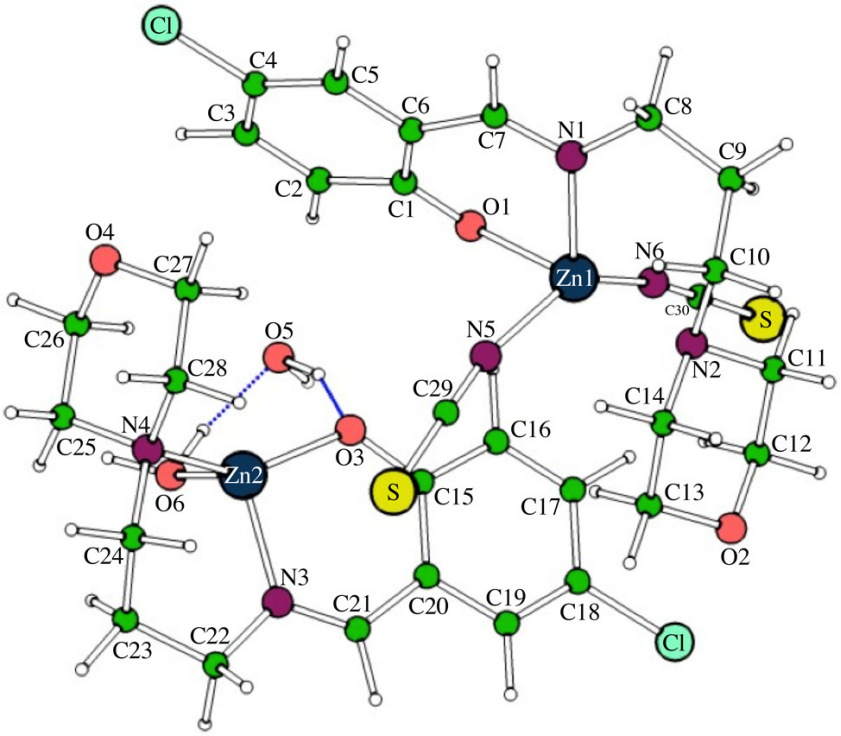
$[Zn(L^1H)_2](ClO_4)_2$		$[Zn(L^2H)_2](ClO_4)_2$	
Atoms	^1H	Atoms	^1H
H(C2)	6.94	H(C2)	6.54
H(C3)	7.36	H(C3)	7.18
H(C5)	7.11	H(C5)	7.08
H(C7)	8.06	H(C7)	8.38
H(C8)	4.05, 4.17	H(C8)	3.39, 4.98
H(C9)	3.37, 3.42	H(C9)	1.74, 2.21
H(C10)	2.80, 3.32	H(C10)	3.00, 3.26
H(C11)	3.89, 4.02	H(C11)	3.07, 3.30
H(C12)	3.80, 3.56	H(C12)	3.76, 4.15

H(C13)	0.62, 3.80	H(C13)	4.09, 3.65
H(C15)	6.91	H(C14)	2.93, 3.11
H(C16)	7.32	H(C16)	6.60
H(C18)	7.28	H(C17)	7.21
H(C20)	8.70	H(C19)	7.03
H(C21)	3.85, 3.87	H(C21)	8.62
H(C22)	3.30, 3.61	H(C22)	3.75, 4.81
H(C23)	3.03, 3.28	H(C23)	1.63, 2.03
H(C24)	3.76, 4.10	H(C24)	2.83, 4.21
H(C25)	3.69, 3.91	H(C25)	2.95, 3.47
H(C26)	0.65, 3.09	H(C26)	3.77, 4.09
H(N2)	8.90	H(C27)	3.69, 4.20
H(N4)	4.22	H(C28)	2.95, 3.20
		H(N2)	4.16
		H(N4)	4.21

$[Zn(L^1)(H_2O)_2][Zn(L^1)(SCN)_2]$

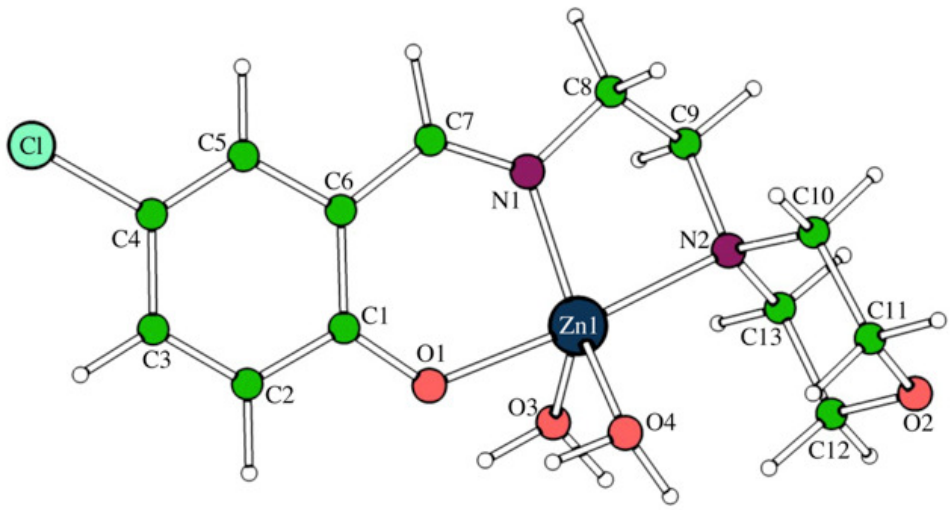


$[Zn(L^2)(H_2O)_2][Zn(L^2)(SCN)_2]$

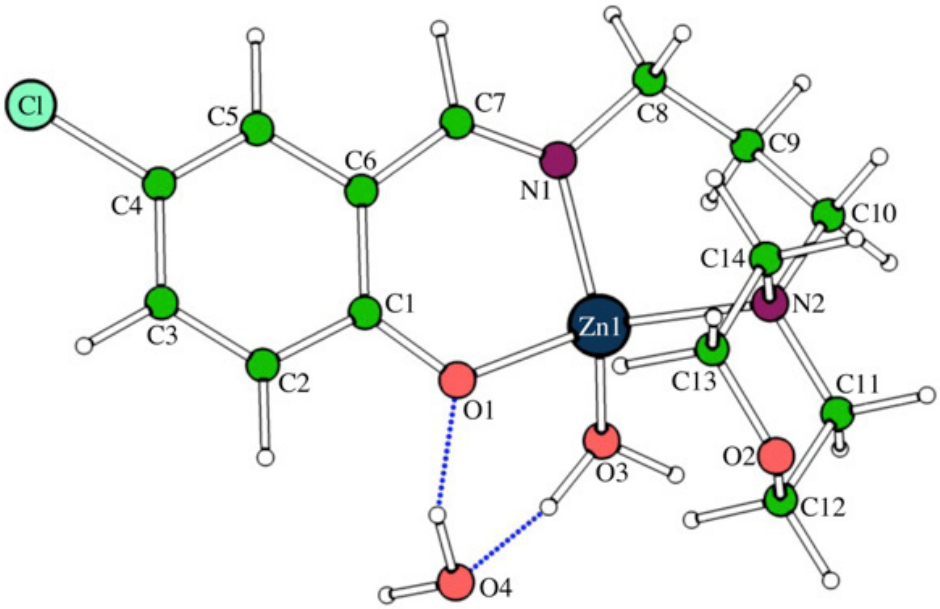


$[Zn(L^1)(H_2O)_2][Zn(L^1)(SCN)_2]$		$[Zn(L^2)(H_2O)_2][Zn(L^2)(SCN)_2]$	
Atoms	^1H	Atoms	^1H
H(C2)	6.64	H(C2)	7.20
H(C3)	7.08	H(C3)	7.07
H(C5)	6.91	H(C5)	6.83
H(C7)	8.13	H(C7)	7.94
H(C8)	3.29, 3.91	H(C8)	3.31, 3.66
H(C9)	2.38, 2.93	H(C9)	1.55, 2.21
H(C10)	2.50, 3.23	H(C10)	2.29, 2.40
H(C11)	4.13, 4.37	H(C11)	1.71, 3.65
H(C12)	3.69, 4.22	H(C12)	4.01, 4.33
H(C13)	2.05, 2.99	H(C13)	2.71, 3.40
H(C15)	7.67	H(C14)	1.85, 2.74
H(C16)	7.17	H(C16)	8.19
H(C18)	6.99	H(C17)	8.14
H(C20)	8.14	H(C19)	7.05
H(C21)	3.23, 3.92	H(C21)	8.02
H(C22)	2.85, 2.71	H(C22)	3.64, 3.84
H(C23)	2.32, 3.37	H(C23)	1.81, 2.09
H(C24)	3.88, 4.18	H(C24)	2.81, 3.09
H(C25)	4.03, 4.92	H(C25)	2.32, 3.45
H(C26)	2.80, 3.76	H(C26)	3.85, 4.27
H(O5)	5.27, 12.03	H(C27)	3.00, 3.55
H(O6)	0.98, 5.17	H(C28)	2.34, 4.48
		H(O5)	2.81, 7.60
		H(O6)	2.66, 9.73

$[Zn(L^1)(H_2O)_2]^{1+}$

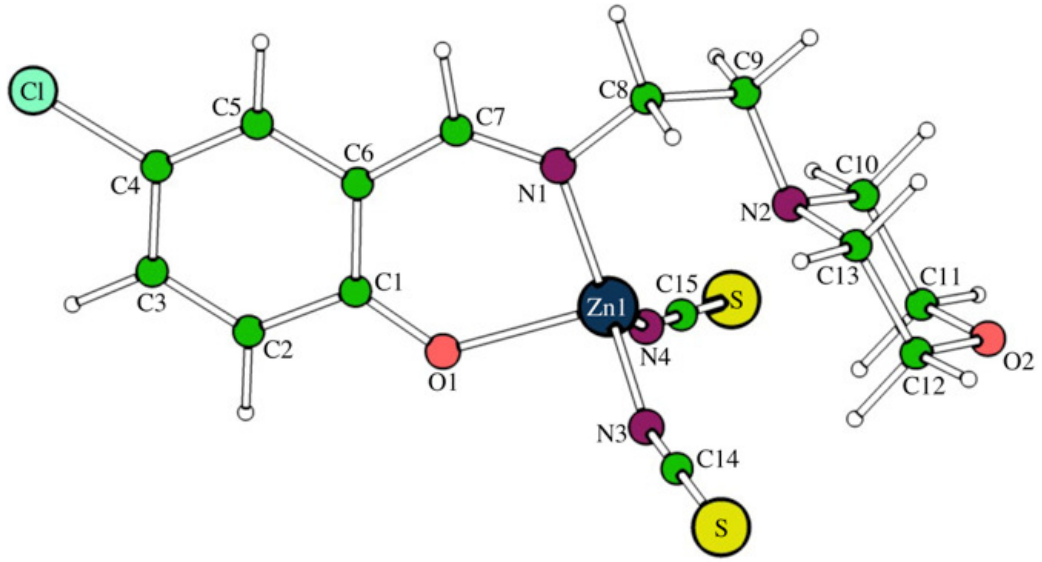


$[Zn(L^2)(H_2O)_2]^{1+}$

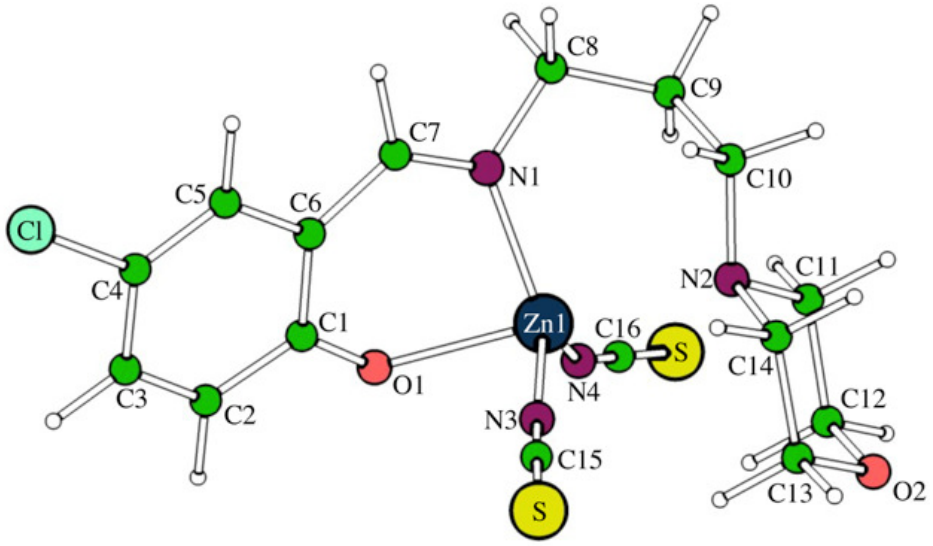


$[Zn(L^1)(H_2O)_2]^{1+}$		$[Zn(L^2)(H_2O)_2]^{1+}$	
Atoms	^1H	Atoms	^1H
H(C2)	6.65	H(C2)	6.81
H(C3)	7.11	H(C3)	7.22
H(C5)	6.94	H(C5)	7.06
H(C7)	8.22	H(C7)	8.11
H(C8)	3.33, 4.18	H(C8)	3.83, 3.93
H(C9)	2.79, 2.95	H(C9)	2.08, 2.09
H(C10)	2.70, 2.94	H(C10)	3.07, 3.18
H(C11)	3.57, 4.25	H(C11)	2.82, 2.90
H(C12)	3.61, 4.11	H(C12)	3.77, 4.30
H(C13)	2.37, 3.43	H(C13)	3.92, 4.02
H(O3)	3.18, 3.23	H(C14)	2.71, 3.14
H(O4)	3.44, 3.94	H(O3)	3.30, 10.66
		H(O4)	2.80, 7.33

$[Zn(L^1)(SCN)_2]^{1-}$

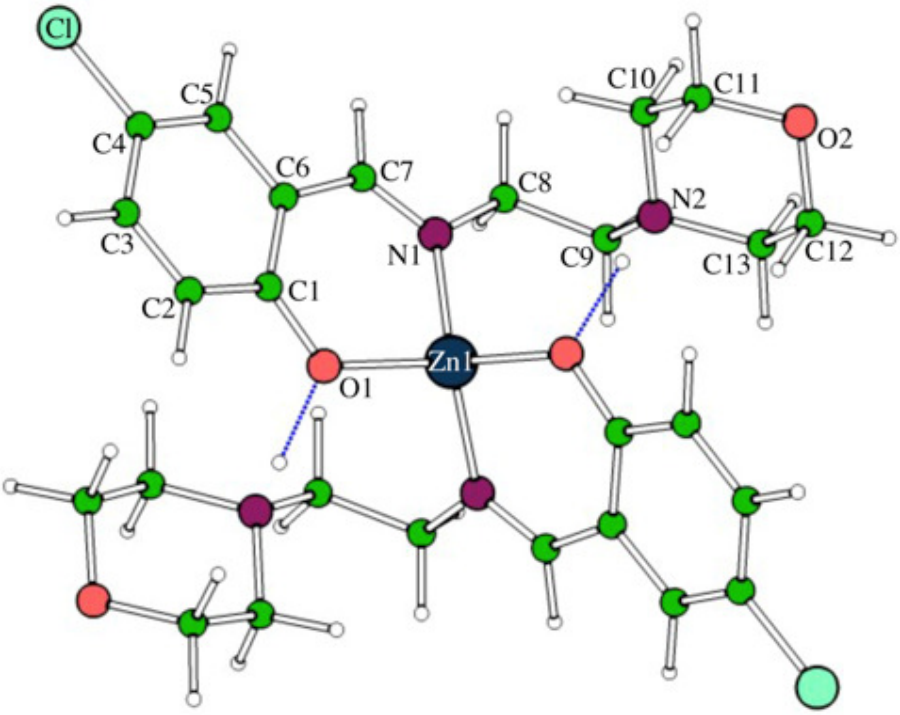

Cl
C5
C6
C7
C8
C9
C4
N1
C10
N2
C13
C11
C3
C1
Zn1
C15
S
C2
O1
N4
O2
C12
N3
C14
S

$[Zn(L^2)(SCN)_2]^{1-}$

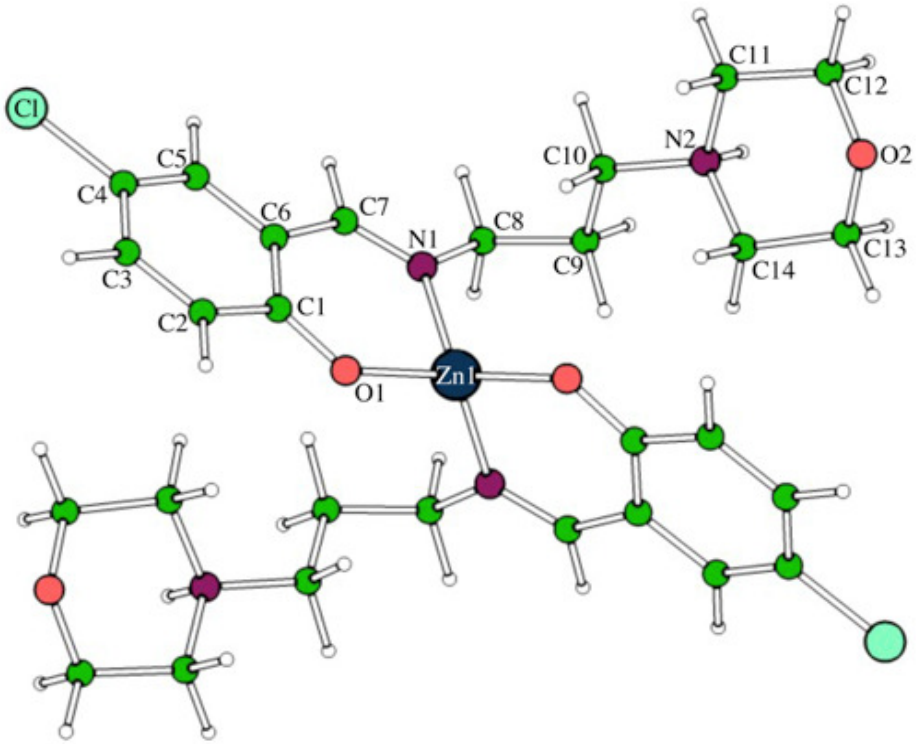

C8
C9
C7
N1
C10
C5
C6
Cl
N2
C11
C4
C1
Zn1
C16
S
C14
O1
N4
C3
C2
N3
C12
C15
C13
O2
S

$[Zn(L^1)(SCN)_2]^{1-}$		$[Zn(L^2)(SCN)_2]^{1-}$	
Atoms	^1H	Atoms	^1H
H(C2)	6.41	H(C2)	6.40
H(C3)	6.95	H(C3)	6.94
H(C5)	6.79	H(C5)	6.84
H(C7)	7.95	H(C7)	8.03
H(C8)	2.99, 4.23	H(C8)	3.34, 3.81
H(C9)	2.47, 2.63	H(C9)	1.68, 2.22
H(C10)	2.34, 2.99	H(C10)	2.37, 2.58
H(C11)	3.96, 4.21	H(C11)	1.82, 3.69
H(C12)	4.07, 4.45	H(C12)	4.04, 4.26
H(C13)	2.04, 3.48	H(C13)	3.88, 4.36
		H(C14)	2.13, 3.06

$[Zn(L^1H)_2]^{2+}$



$[Zn(L^2H)_2]^{2+}$



$[Zn(L^1H)_2]^{2+}$		$[Zn(L^2H)_2]^{2+}$	
Atoms	^1H	Atoms	^1H
H(C2)	5.92	H(C2)	6.64
H(C3)	4.36	H(C3)	7.27
H(C5)	5.93	H(C5)	7.05
H(C7)	7.14	H(C7)	8.12
H(C8)	3.75, 3.48	H(C8)	4.18, 3.35
H(C9)	2.84, 2.82	H(C9)	2.16, 1.76
H(C10)	2.91, 2.60	H(C10)	3.16, 2.97
H(C11)	4.09, 3.92	H(C11)	3.26, 3.08
H(C12)	4.36, 3.97	H(C12)	4.13, 3.75
H(C13)	2.95, 2.86	H(C13)	3.99, 3.60
H(N2)	10.68	H(C14)	2.91, 2.76
		H(N2)	4.14

HL[1]		**HL[2]**	
Atoms	^{1}H	Atoms	^{1}H
H(C2)	6.78	H(C2)	6.80
H(C3)	7.12	H(C3)	7.12
H(C5)	7.17	H(C5)	7.09
H(C7)	8.04	H(C7)	8.92
H(C8)	3.51, 3.69	H(C8)	3.58, 3.87
H(C9)	2.27, 2.52	H(C9)	1.63, 1.99
H(C10)	2.26, 2.50	H(C10)	2.04, 2.23
H(C11)	3.48, 3.76	H(C11)	1.79, 2.90
H(C12)	3.71, 3.92	H(C12)	3.84, 3.92
H(C13)	1.98, 3.15	H(C13)	3.82, 3.84
H(O1)	16.44	H(C14)	2.08, 2.17
		H(O1)	16.46