

Electronic Supplementary Information

Combined experimental and theoretical rationalization on zinc(II) mediated unusual conversion of 18-membered Schiff-base macrocycle to 18-membered imine-amine macrocycle having imidazolidine side rings: investigation of their bio-relevant catalytic activities

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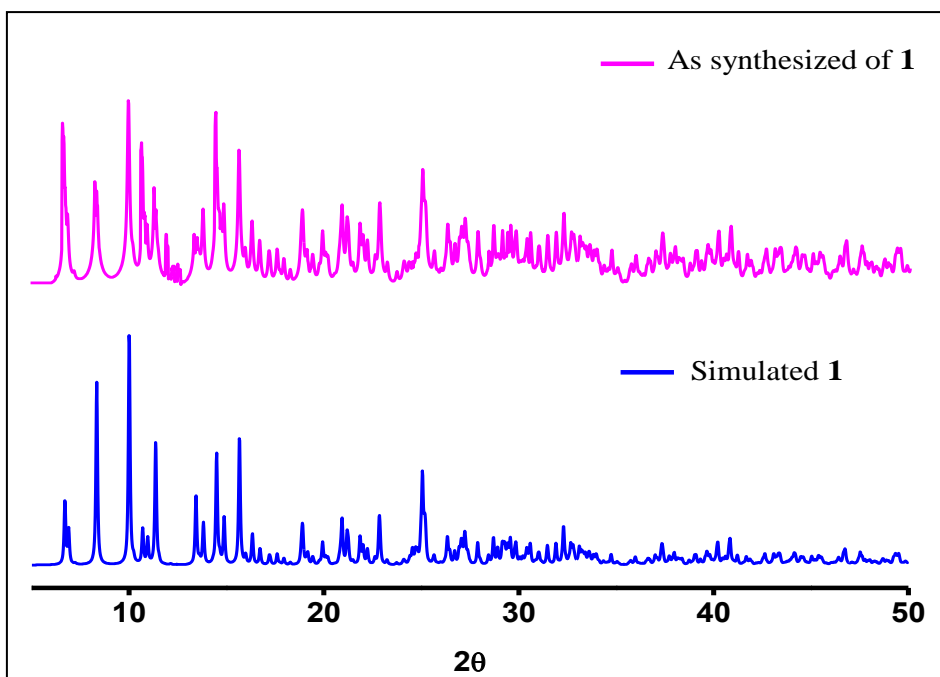


Fig. S1 PXRD pattern of simulated complex **1**, as synthesized **1** collected under air.

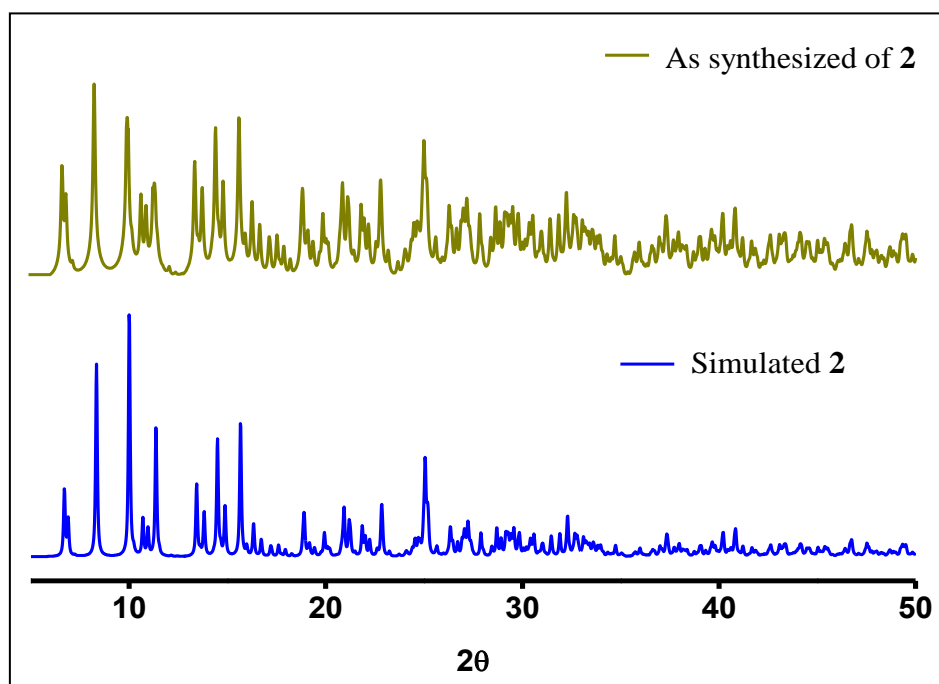


Fig. S2 PXRD pattern of simulated complex **2**, as synthesized **2** collected under air.

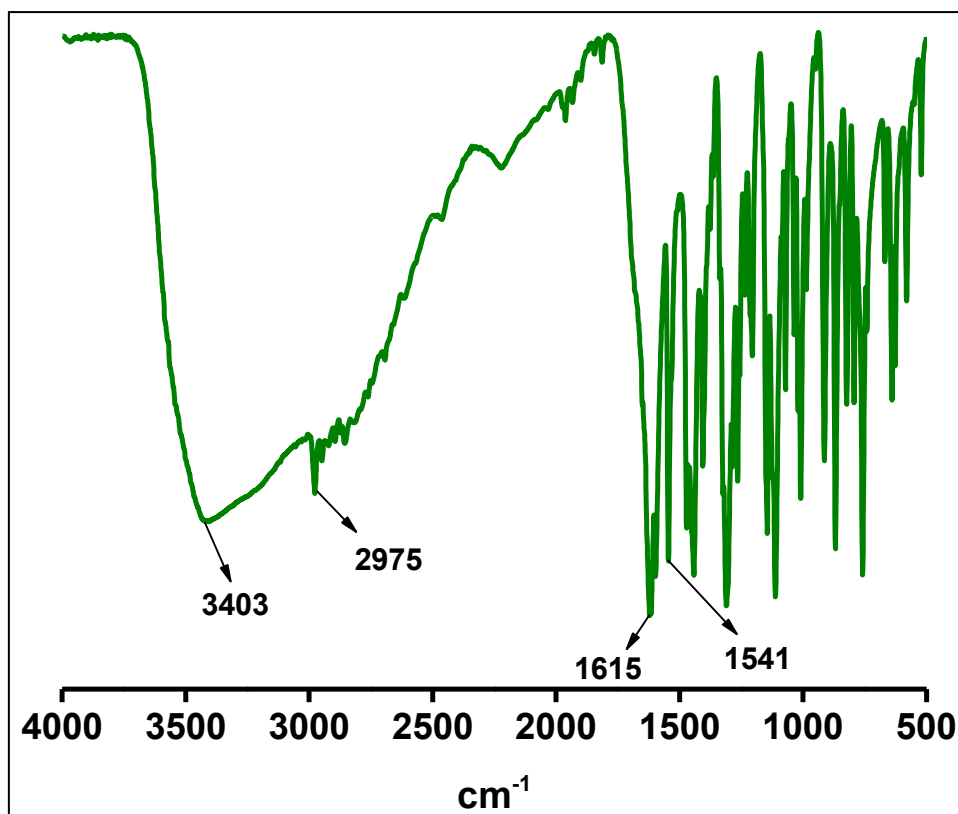


Fig. S3 FT-IR Spectrum of Ligand (H₂L).

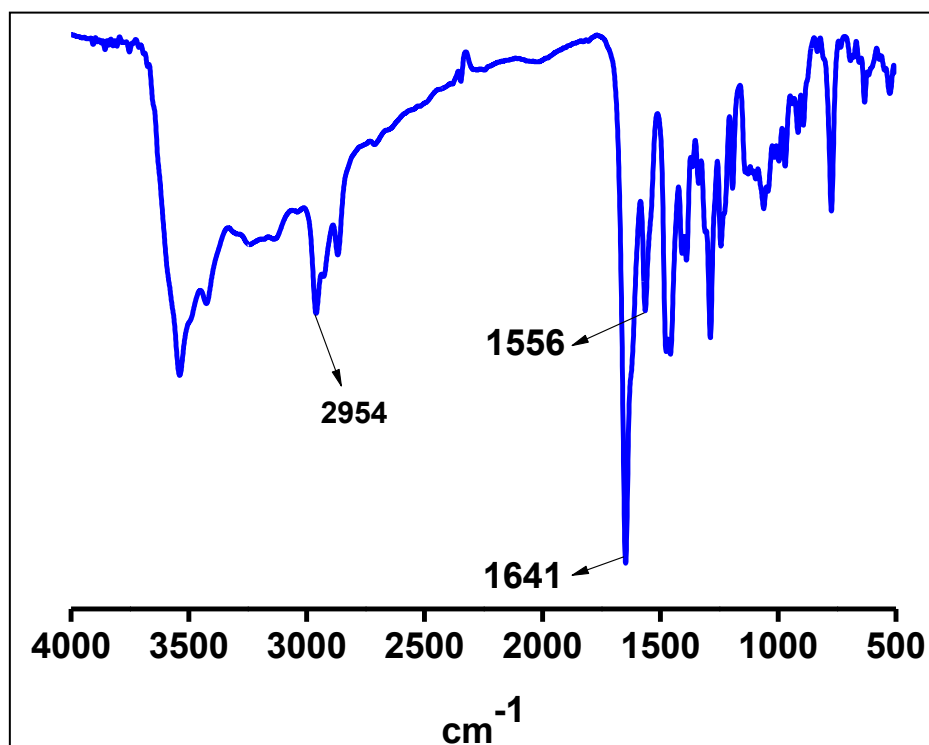


Fig. S4 FT-IR Spectrum of complex 1.

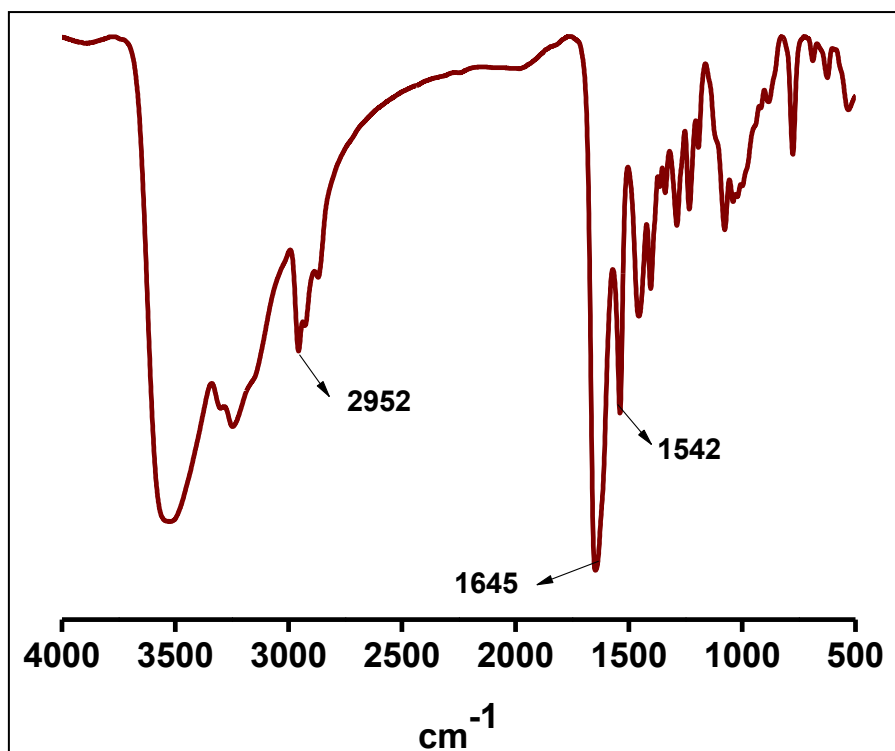


Fig. S5 FT-IR Spectrum of complex 2.

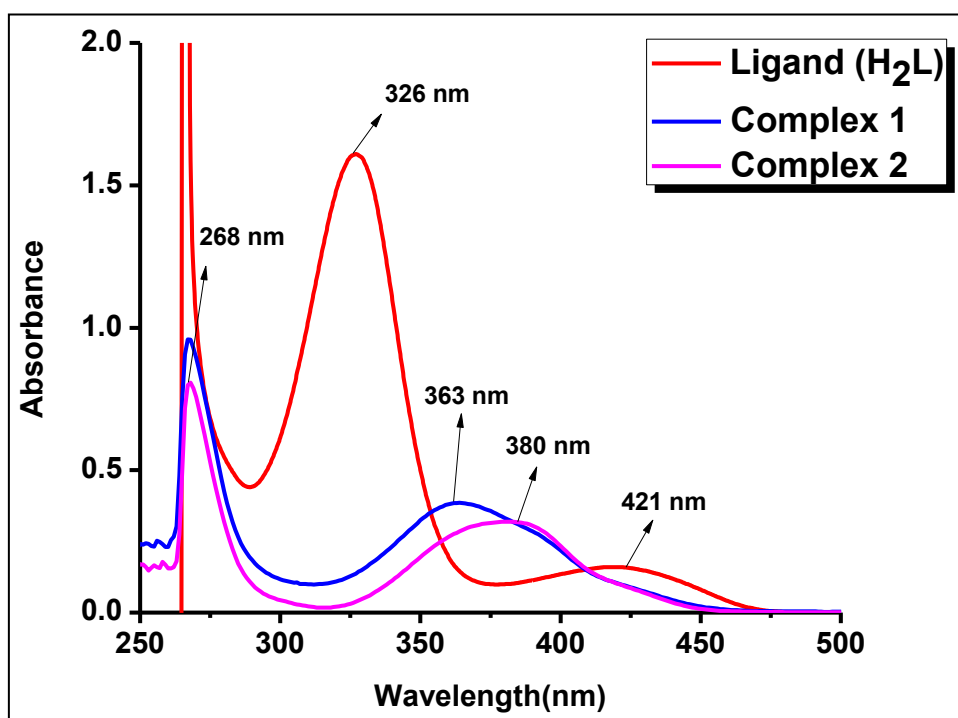


Fig. S6 UV-Vis spectrum of ligand H_2L and complex (1-2) in DMF medium at 25 °C (zoom out) in the wavelength range of 250-500 nm.

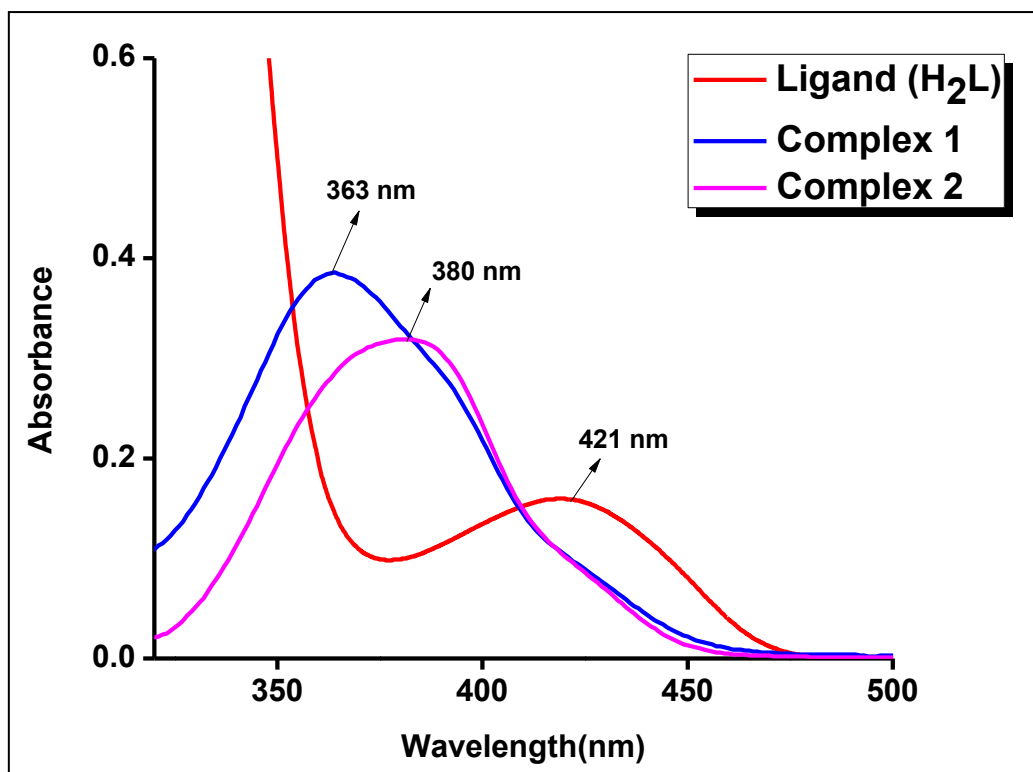


Fig. S7 UV-Vis spectrum of ligand H_2L and complex (1-2) in DMF medium at 25 °C (zoom in) in the wavelength range of 320-500 nm.

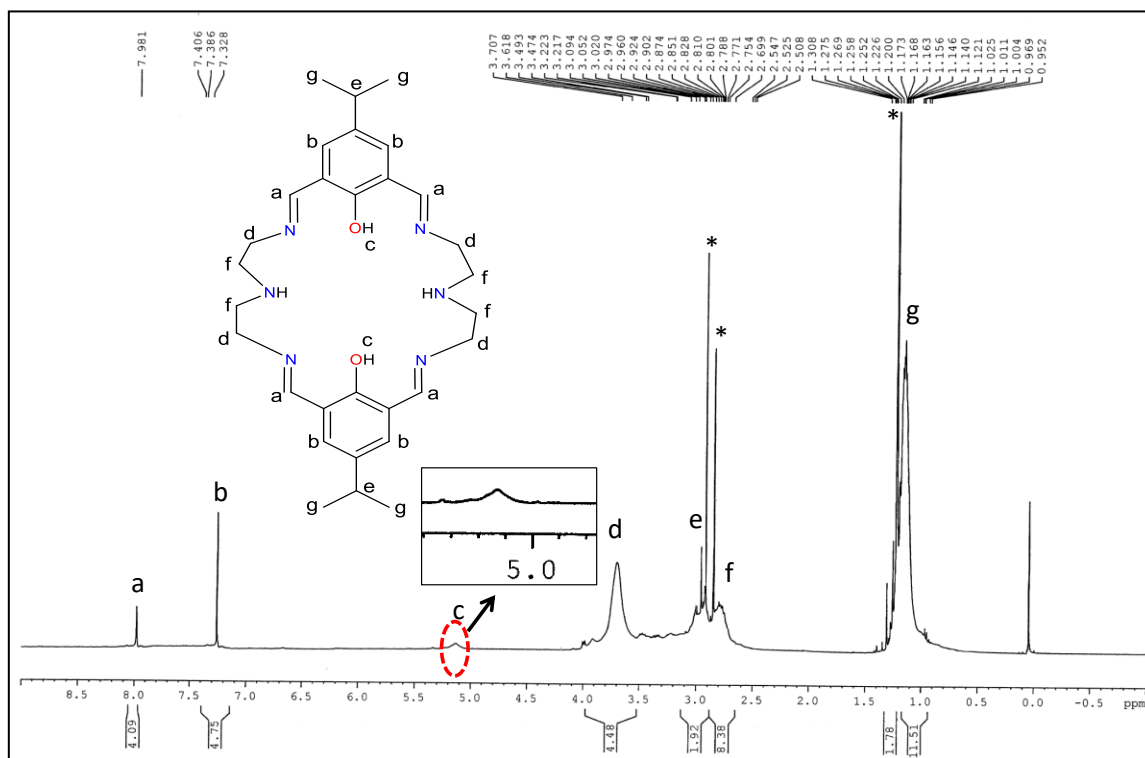


Fig. S8 1H -NMR spectra of ligand H_2L in $CDCl_3$.

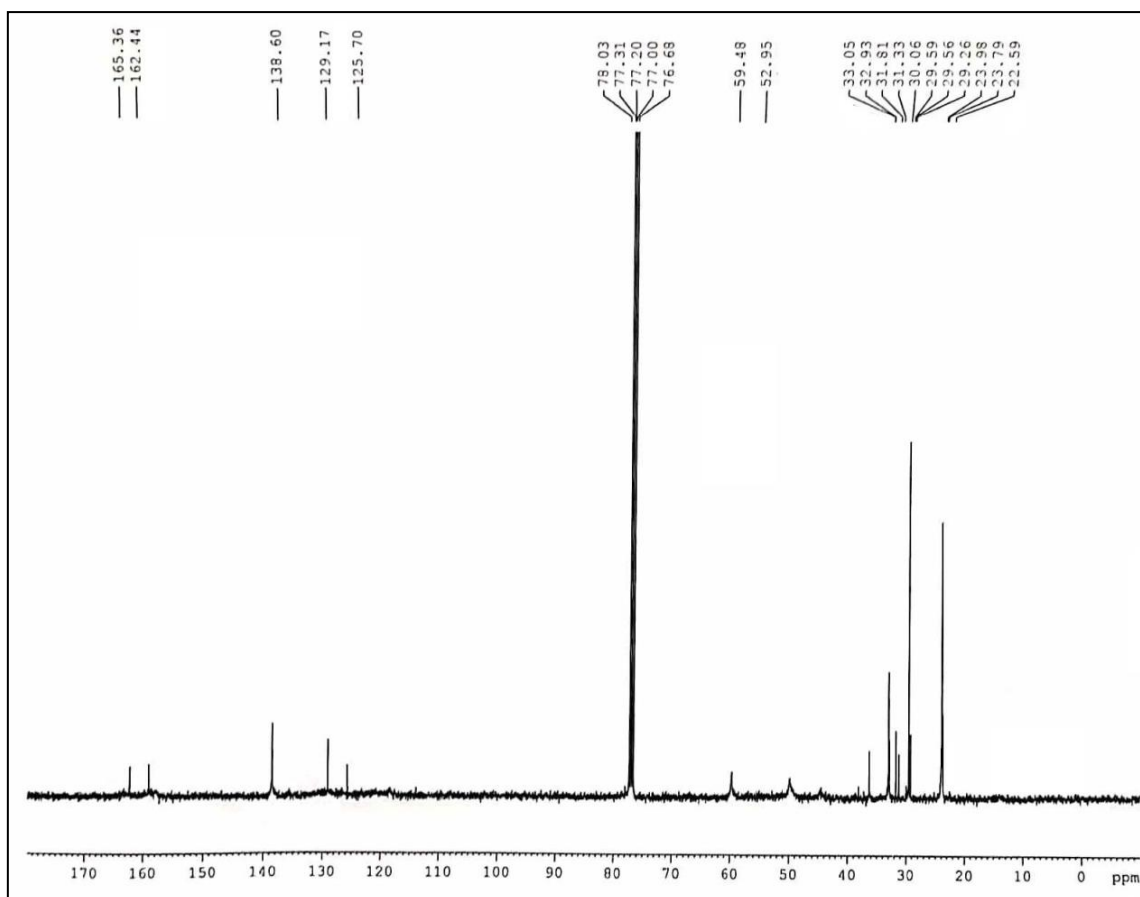


Fig. S9 ^{13}C -NMR spectra of ligand H_2L in CDCl_3 .

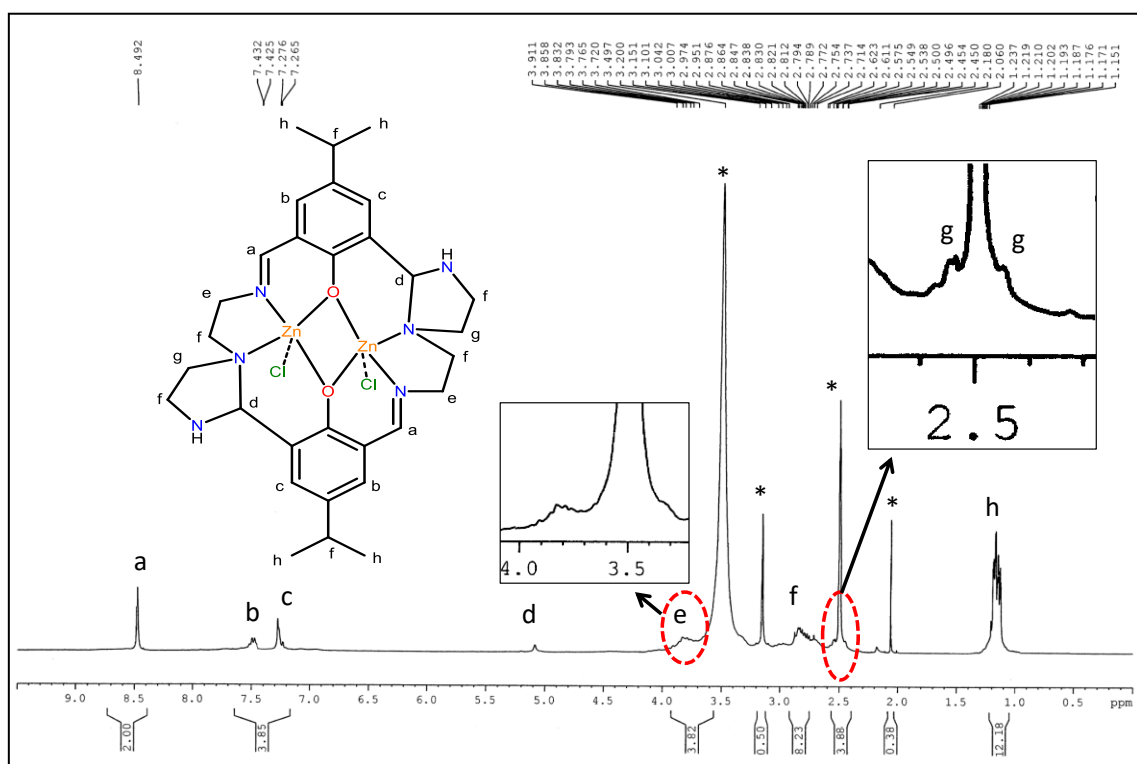


Fig. S10 ^1H -NMR spectra of complex **1** in d_6 -DMSO.

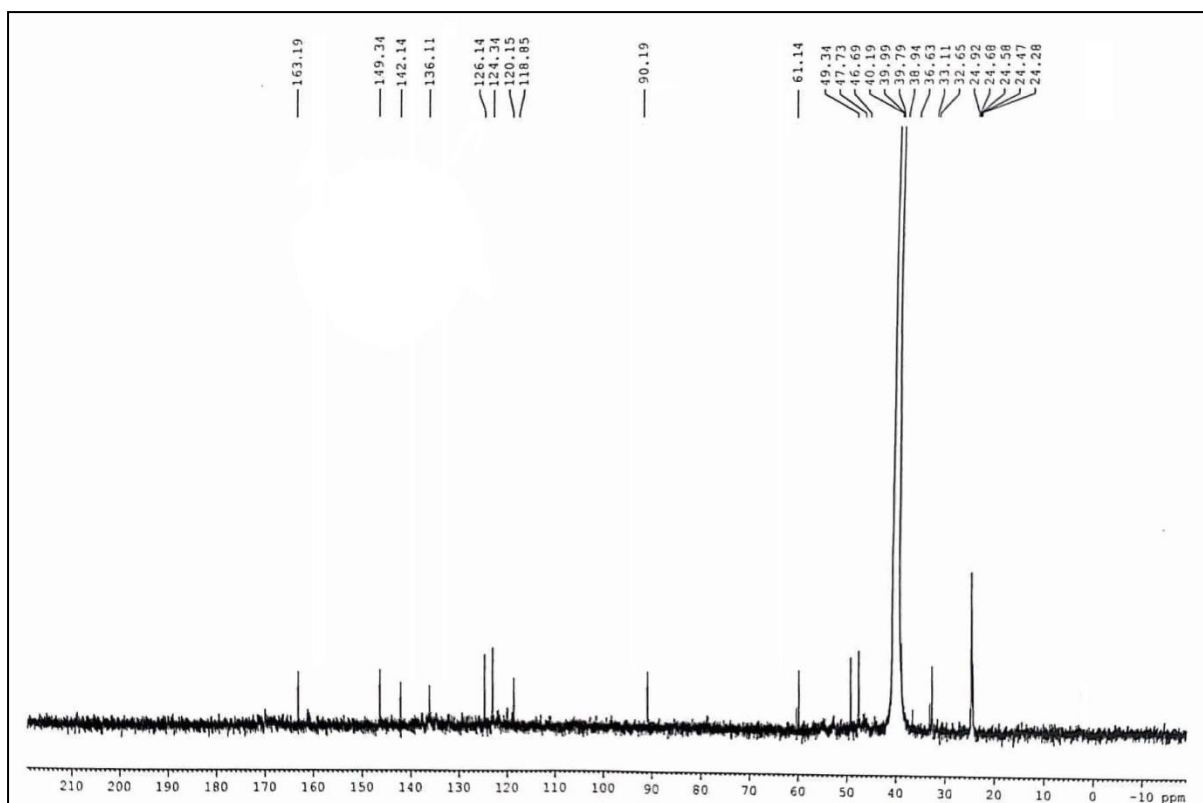


Fig. S11 ^{13}C -NMR spectra of complex **1** in d_6 -DMSO.

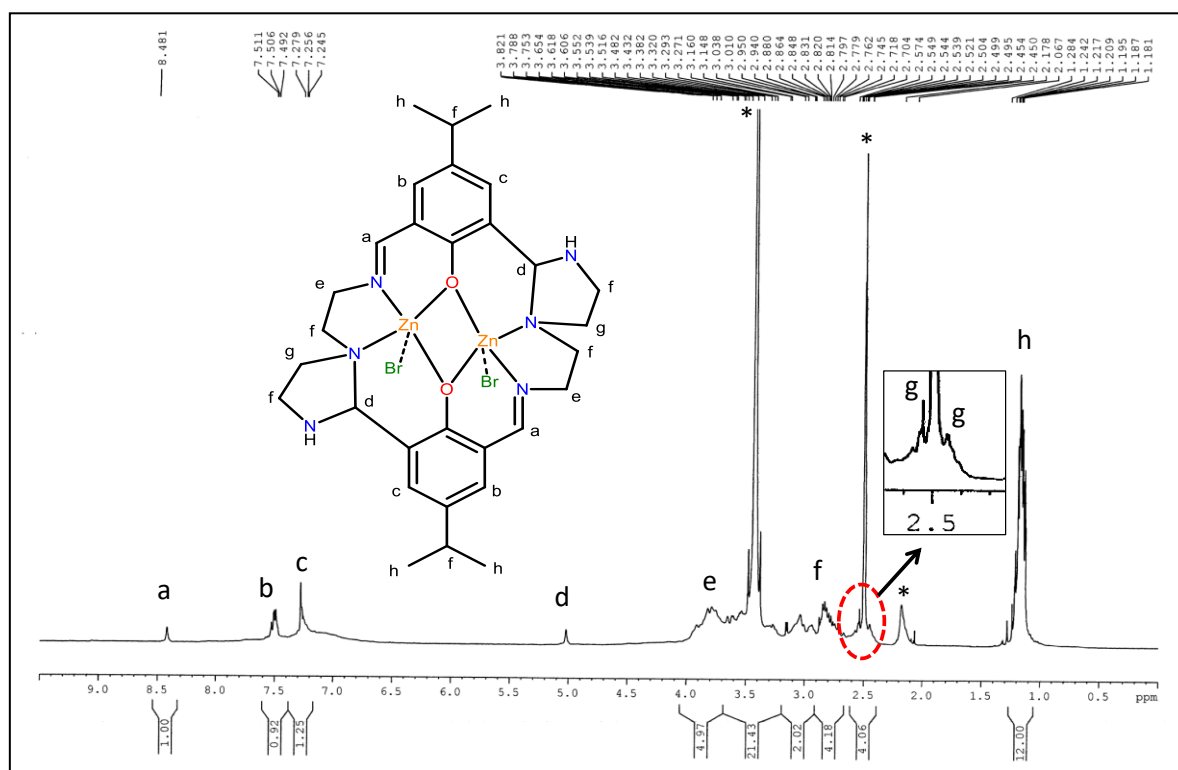


Fig. S12 ^1H -NMR spectra of complex **2** in d_6 -DMSO.

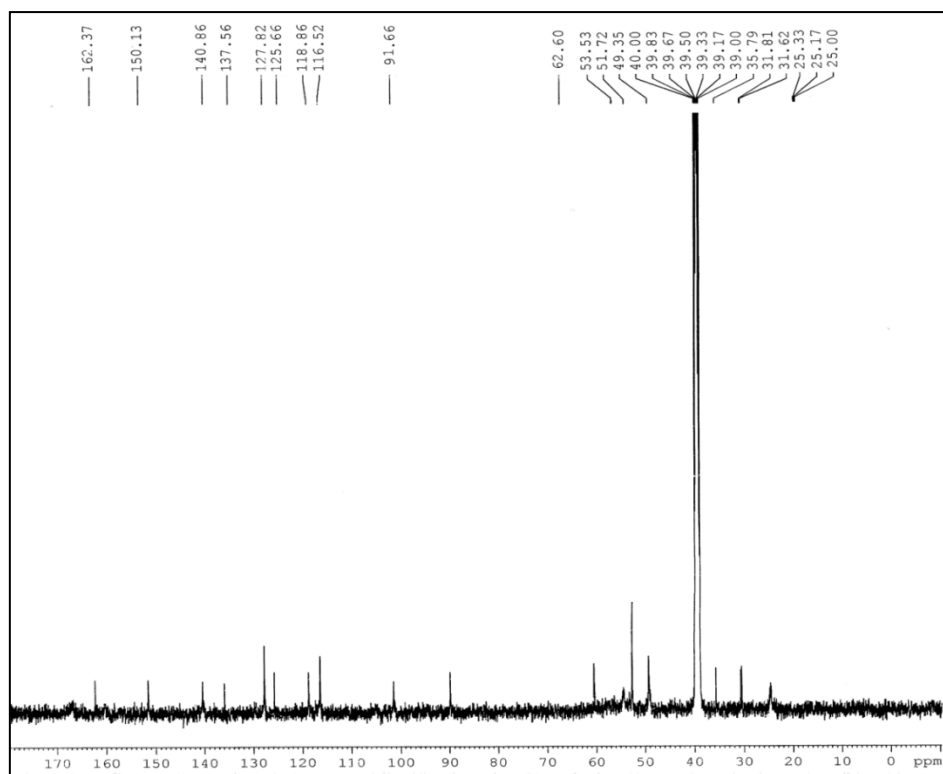


Fig. S13 ^{13}C -NMR spectra of complex **2** in d_6 -DMSO.

Table S1 Coordination bond lengths (\AA) and angles ($^\circ$) for complex **1**.

Bond Distance (\AA)			
Zn1 – Cl1	2.2427(16)	Zn2 – Cl2	2.2463(15)
Zn1 – O1	2.022(3)	Zn2 – N4	2.003(3)
Zn1 – O2	2.148(3)	Zn2 – N5	2.264(3)
Zn1 – N1	2.213(3)	Zn3 – Cl3	2.2729(19)
Zn1 – N2	2.026(3)	Zn3 – Cl5	2.2407(16)
Zn2 – O1	2.149(3)	Zn3 – Cl4	2.214(2)
Zn2 – O2	2.011(3)	Zn3 – N3	2.096(3)
Bond Angles ($^\circ$)			
Cl1 – Zn1 – O1	113.30(7)	N1 – Zn1 – N2	82.29(12)
Cl1 – Zn1 – O2	97.35(7)	N4 – Zn2 – N5	81.40(11)
Cl1 – Zn1 – N1	104.32(8)	Cl2 – Zn2 – O1	99.60(7)
Cl1 – Zn1 – N2	117.40(8)	Cl2 – Zn2 – O2	115.31(7)
O1 – Zn1 – O2	81.74(11)	Cl2 – Zn2 – N4	119.45(10)
O1 – Zn1 – N1	90.35(11)	Cl2 – Zn2 – N5	100.84(9)
O1 – Zn1 – N2	129.04(10)	O1 – Zn2 – O2	81.96(10)
O2 – Zn1 – N1	158.32(10)	O1 – Zn2 – N4	88.33(11)
O1 – Zn2 – N5	159.55(10)	Cl3 – Zn3 – Cl4	109.58(7)
O2 – Zn2 – N4	125.24(12)	Cl3 – Zn3 – Cl5	108.21(5)
O2 – Zn2 – N5	89.57(11)	Cl3 – Zn3 – N3	104.02(9)
O2 – Zn1 – N2	87.09(11)	Cl4 – Zn3 – Cl5	112.80(7)
Cl4 – Zn3 – N3	106.19(11)	Zn1 – O2 – Zn2	94.52(12)
Cl5 – Zn3 – N3	115.60(9)	Zn1 – O1 – Zn2	94.18(11)

Table S2 Coordination bond lengths (Å) and angles (°) for complex **2**.

Bond Distance (Å)			
Zn1 – Br1	2.3730(18)	Zn1 – N1	2.235(8)
Zn2 – Br2	2.3864(18)	Zn1 – N2	2.035(7)
Zn1 – O1	2.016(6)	Zn2 – O2	2.007(6)
Zn1 – O2	2.171(6)	Zn2 – N4	2.006(7)
Zn2 – O1	2.169(6)	Zn2 – N5	2.282(8)
Zn3 – Br3	2.379(2)	Zn3 – Br5	2.411(2)
Zn3 – Br4	2.348(2)	Zn3 – N3	2.079(9)
Bond Angles (°)			
Br1 – Zn1 – O1	115.24(16)	O2 – Zn1 – N2	86.6(3)
Br1 – Zn1 – O2	98.35(15)	N1 – Zn1 – N2	82.4(3)
Br1 – Zn1 – N1	103.98(18)	Br2 – Zn2 – O1	100.32(16)
Br1 – Zn1 – N2	115.57(19)	Br2 – Zn2 – O2	116.95(16)
O1 – Zn1 – O2	81.5(2)	Br2 – Zn2 – N4	118.1(2)
O1 – Zn1 – N1	90.3(2)	Br2 – Zn2 – N5	101.30(15)
O1 – Zn1 – N2	128.9(2)	O1 – Zn2 – O2	81.8(2)
O2 – Zn1 – N1	157.6(2)	O1 – Zn2 – N4	88.1(3)
O1 – Zn2 – N5	158.4(2)	Br3 – Zn3 – Br4	112.08(7)
O2 – Zn2 – N4	124.9(3)	Br3 – Zn3 – Br5	108.16(6)
O2 – Zn2 – N5	89.1(2)	Br3 – Zn3 – N3	116.3(2)
N4 – Zn2 – N5	81.1(3)	Br4 – Zn3 – Br5	109.78(7)
Br4 – Zn3 – N3	105.6(2)	Zn1 – O2 – Zn2	94.3(2)
Br5 – Zn3 – N3	104.5(2)	Zn1 – O1 – Zn2	94.1(2)

Table S3 Selected hydrogen bonding distances (Å) and angles (deg) for the complex **1**.

D-H...A	Symmetry	D-H(Å)	D...A(Å)	A...H(Å)	<D-H-A(deg)
O1 -- H1...Cl2	1-x,1-y,-z	0.8500	3.349(3)	2.6100	146.00
O1 -- H1...Cl1	x, y, z	0.8500	3.202(4)	2.3500	177.00
N3 -- H3...O4	x, y, z	0.9800	2.962(6)	2.0300	157.00
O4 -- H4...Cl2	x, y, z	0.8200	3.238(5)	2.4900	153.00
O4 -- H4...O1	x, y, z	0.8200	3.067(5)	2.5800	120.00
N6 -- H6...O1	x, y, z	0.8900	2.736(5)	1.8800	160.00
N6 -- H6...Cl3	x,-1+y,z	0.8900	3.327(5)	2.5300	150.00
C10 -- H10...O4	1-x,1-y,1-z	0.9300	3.496(6)	2.5800	169.00
C14 -- H14...Cl4	x,-1+y,z	0.9700	3.594(7)	2.7600	145.00
C14 -- H14...Cl2	x, y, z	0.9700	3.460(6)	2.7800	127.00
C15 -- H15...Cl5	x,-1+y,z	0.9800	3.629(5)	2.6700	165.00

Table S4 Selected hydrogen bonding distances (Å) and angles (deg) for the complex **2**.

D-H...A	Symmetry	D-H(Å)	D...A(Å)	A...H(Å)	<D-H-A(deg)
N3 -- H3...O3	x, y, z	0.9800	2.989(12)	2.0600	158.00
O3 -- H3...Br2	x, y, z	0.8200	3.357(11)	2.6000	154.00
O4 -- H4...Br2	1-x,1-y,2-z	0.8500	3.505(8)	2.8000	142.00
O4 -- H4...Br1	x, y, z	0.8500	3.335(10)	2.4900	177.00
N6 -- H6...Br5	x,1+y,z	0.8900	3.514(10)	2.7200	149.00
N6 -- H6...O4	x, y, z	0.8900	2.747(12)	1.8900	161.00
C14 -- H14...Br2	x, y, z	0.9700	3.562(12)	2.8600	130.00
C14 -- H14...Br4	x,1+y,z	0.9700	3.688(12)	2.8400	147.00
C15 -- H15...Br3	x,1+y,z	0.9800	3.745(11)	2.8000	163.00

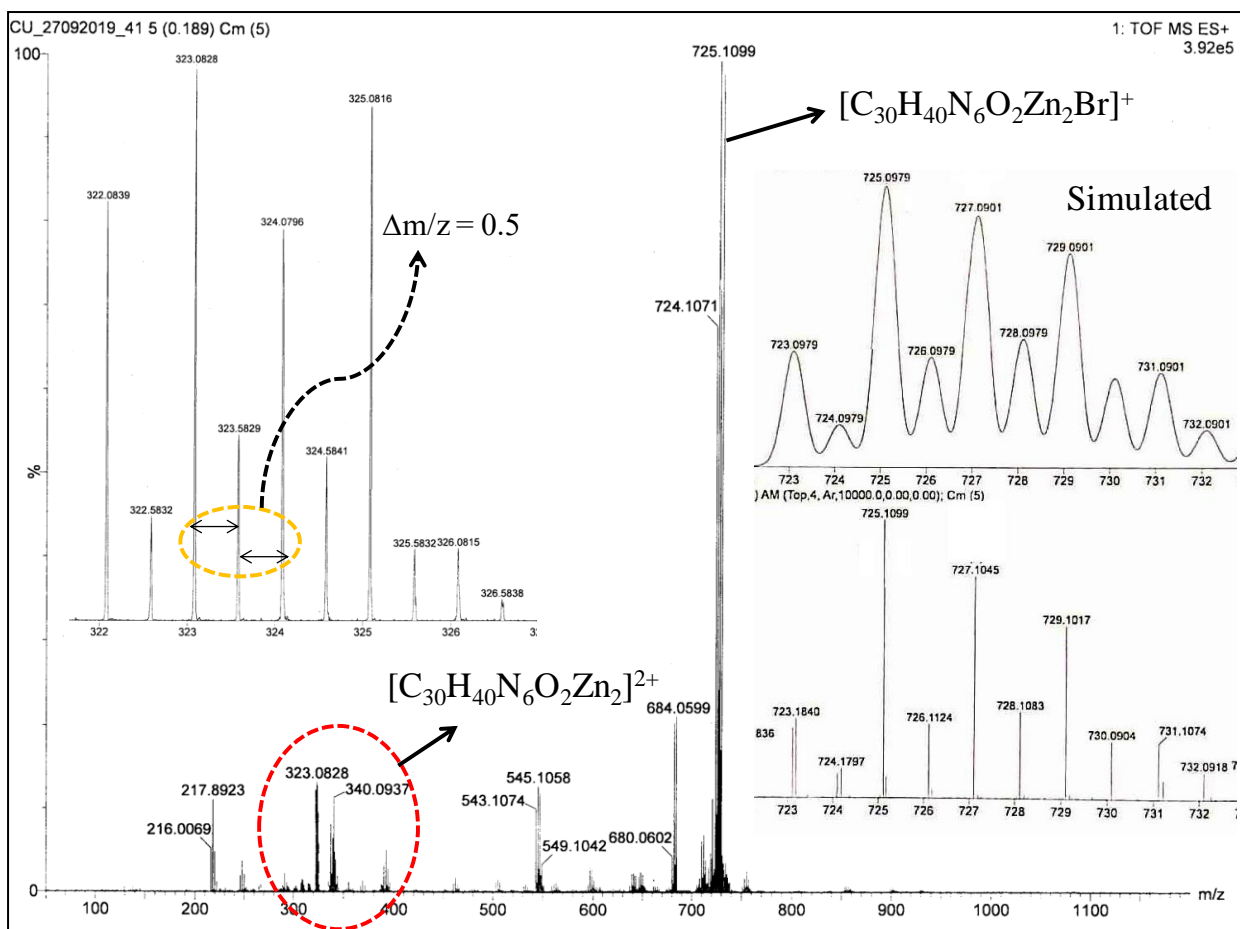


Fig. S14 ESI-MS spectra of complex **2**, inset shows the theoretical simulation and the differences in spacing for the dipositive moiety in solution state.

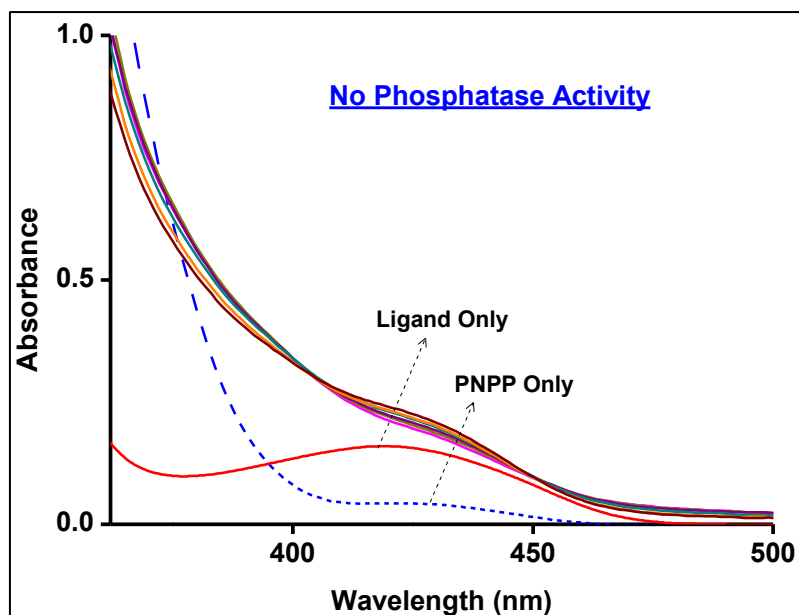


Fig. S15 Wavelength scan of ligand (**H₂L**) and upon the addition of 4-PNPP observed after each 5 min interval.

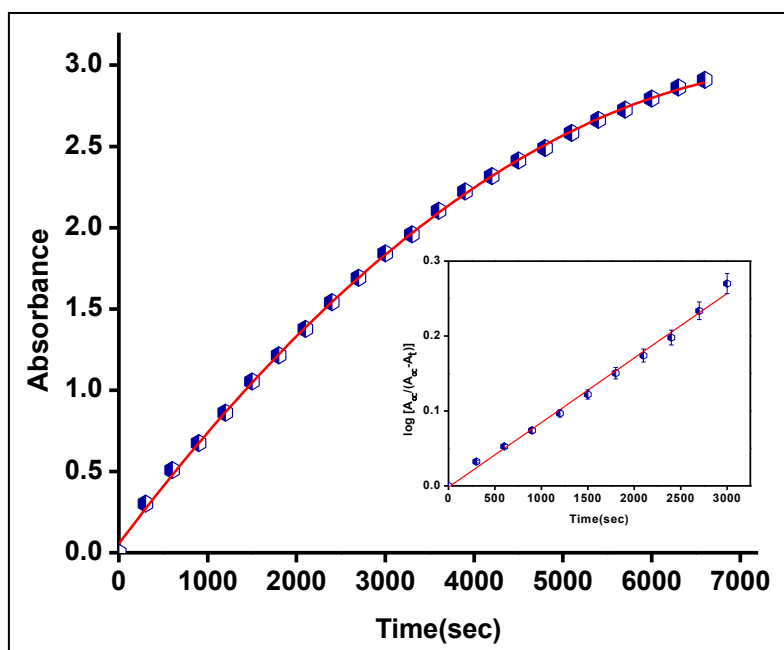


Fig. S16 Absorption profile on addition of 4-PNPP to complex **2** due to the formation of p-nitrophenolate ($\lambda_{\text{max}} = 426 \text{ nm}$) studied for 2 h (Least-squares fit, $R^2 = 0.998$). Inset shows the plot of $\log [A_{\infty}/(A_{\infty} - A_t)]$ versus time for 50 min ($R^2 = 0.993$).

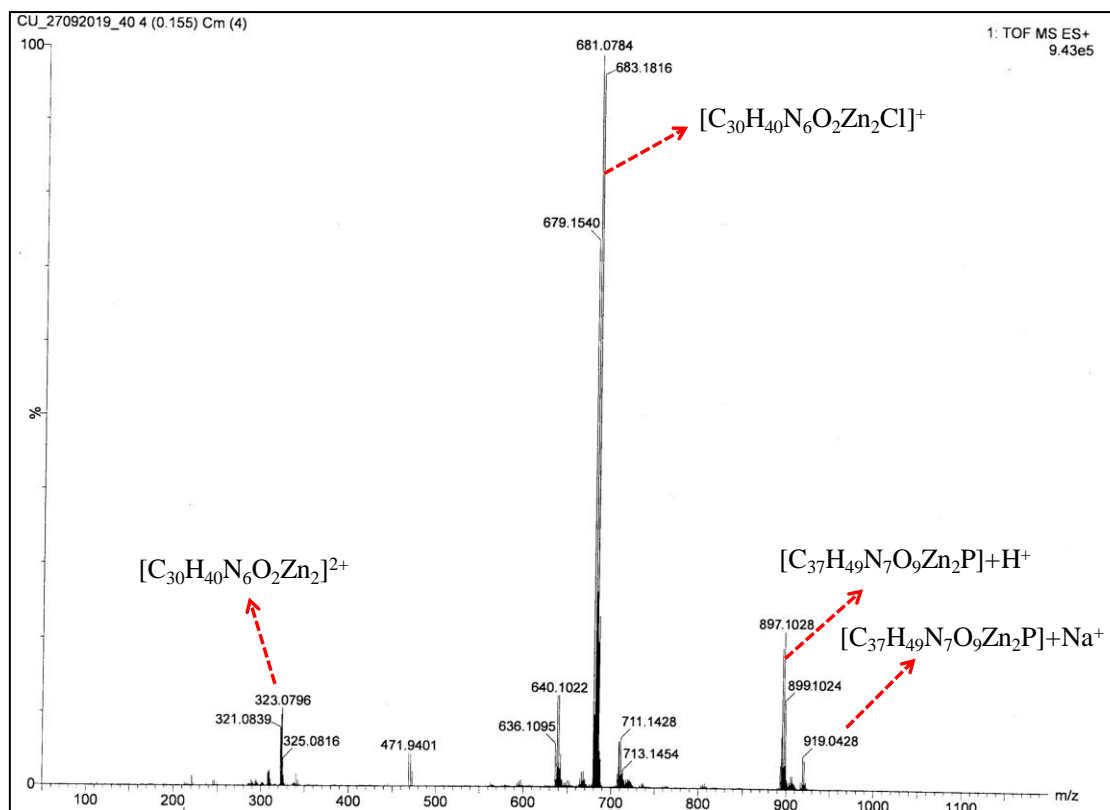


Fig. S17 ESI-MS spectra of reaction mixture of complex **1** and 4-PNPP recorded at 25°C.

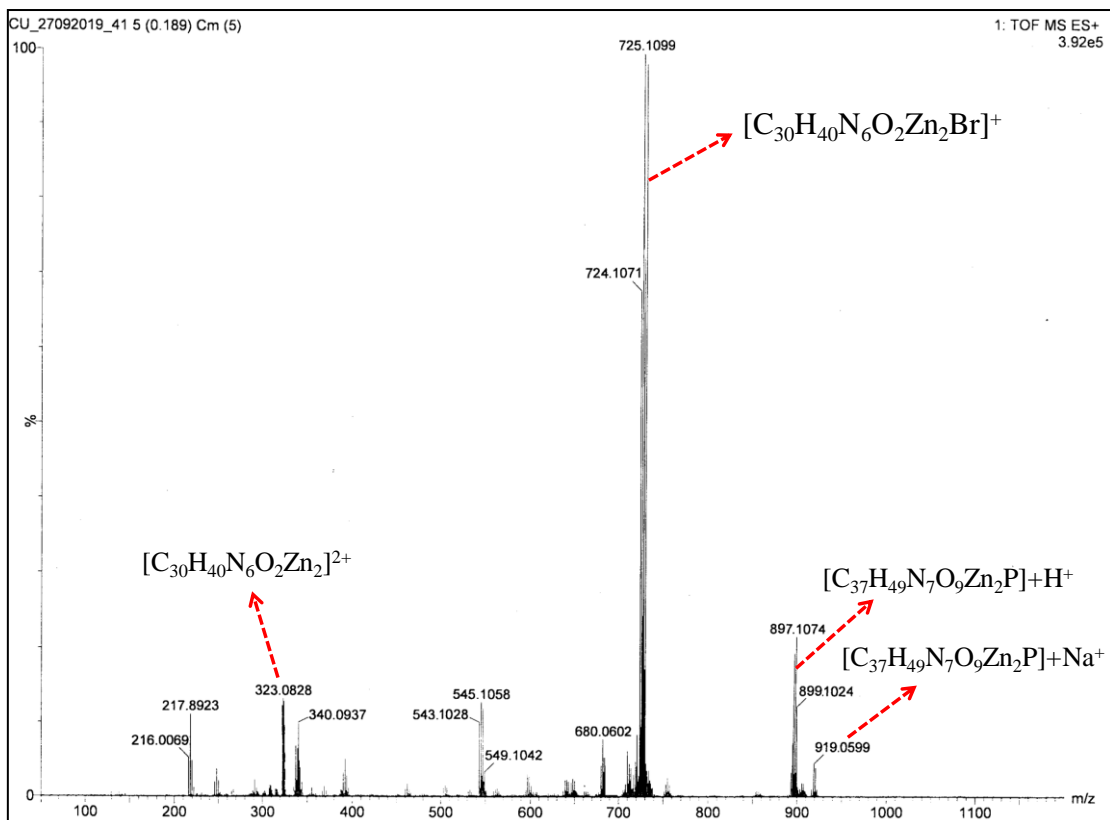


Fig. S18 ESI-MS spectra of reaction mixture of complex **2** and 4-PNPP recorded at 25°C.

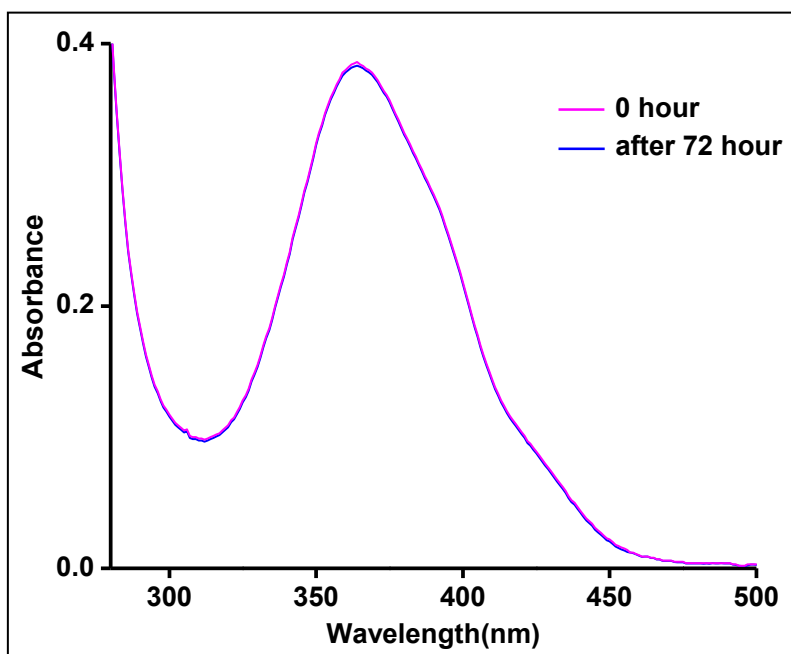


Fig. S19 UV-Vis spectrum of complex **1** at 0 hour and after 72 hours (stability of complex with time) in DMSO medium ($\lambda_{\text{max}} \sim 365$ nm) at 25°C.

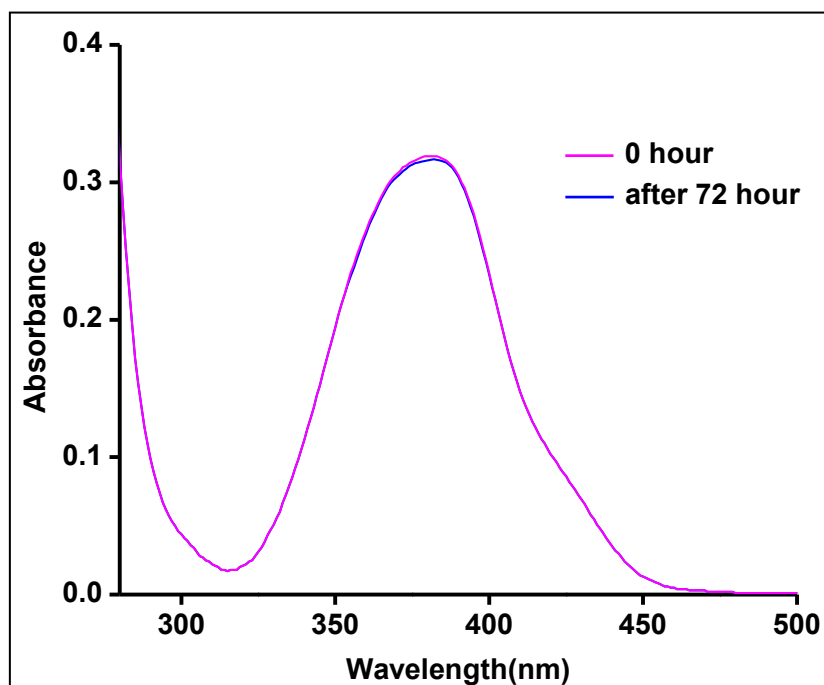


Fig. S20 UV-Vis spectrum of complex **2** at 0 hour and after 72 hours (stability of complex with time) in DMSO medium ($\lambda_{\text{max}} \sim 379$ nm) at 25°C.

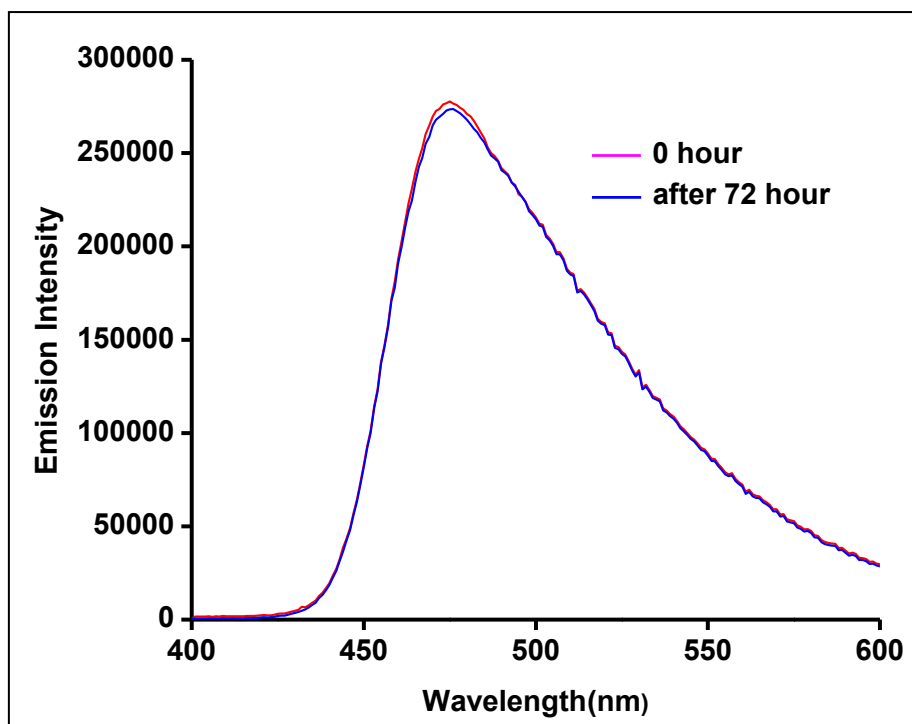


Fig. S21 Fluorescence spectrum of complex **1** at 0 hour and after 72 hours (stability of complex with time) in DMSO medium excited at 448 nm ($\lambda_{\text{max}} \sim 475$ nm) at 25°C.

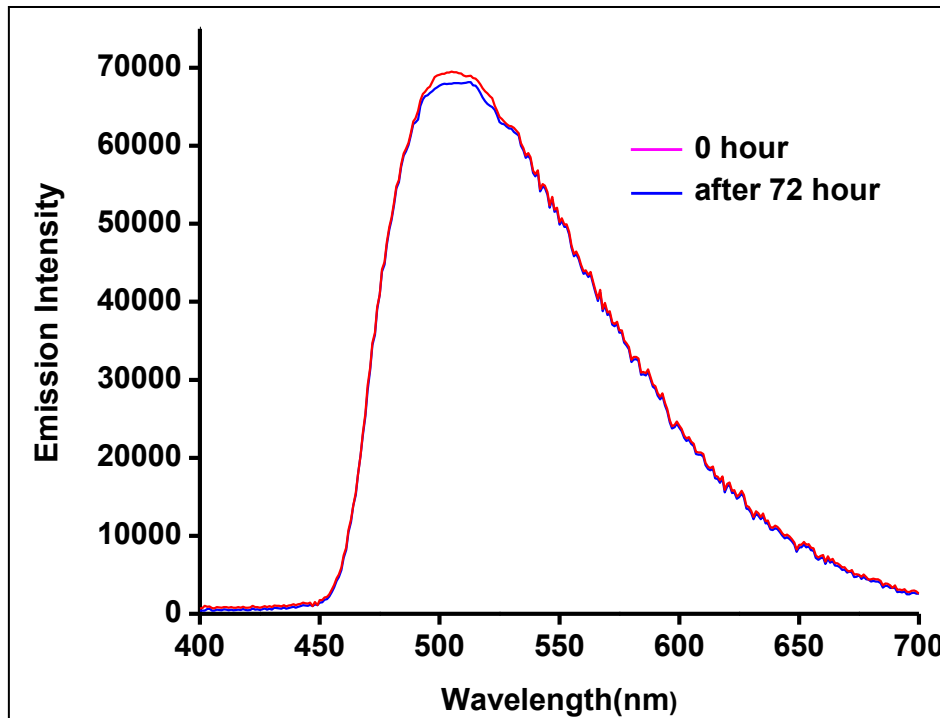


Fig. S22 Fluorescence spectrum of complex **2** at 0 hour and after 72 hours (stability of complex with time) in DMSO medium excited at 452 nm ($\lambda_{\text{max}} \sim 503$ nm) at 25°C.

Table S5 First-order rate constants for the hydrolysis of various phosphate esters by previously reported dinuclear Zn^{II} complexes.^a

Catalyst	Substrate	Solvent	$k_{cat}(s^{-1})$	Ref
[Zn ₂ L]	4-PNPP	MeCN/H ₂ O	476–203	1
[Zn ₂ L ₁ ² X ₂], X= Cl, Br, I	4-PNPP	DMF-H ₂ O (97.5%, v/v)	9.35-8.33	2
[Zn ₂ L ₂ X ₂], X= Cl, Br, I	4-PNPP	DMF-H ₂ O (97.5%, v/v)	9.97-11.62	3
[Zn ₂ (L ₁) ₂ Cl ₂]	4-PNPP	DMF-H ₂ O (97.5%, v/v)	8.94	4
[Zn ₂ (L ₁) ₂ Br ₂]	4-PNPP	DMF-H ₂ O (97.5%, v/v)	13.06	4
[Zn ₂ (L ₂) ₂ (Cl) ₂]	4-PNPP	DMF-H ₂ O (97.5%, v/v)	5.5	5
[Zn ^{II} ₂ (L ²)-(μ-O ₂ CMe) ₂ (MeCN) ₂][PF ₆]	HPNP	MeOH/H ₂ O (33%, v/v)	3.44×10 ⁻⁴	6
[Zn ₂ (L _{2H})(AcO)(H ₂ O)][PF ₆] 0.2H ₂ O	BNPP	MeOH/H ₂ O (1:5)	4.60×10 ⁻⁶	7
[Zn ₂ complex]	HPNP	DMSO/buffered water (1:1)	4.00×10 ⁻⁷	8
[Zn ₂ PBTPA] ⁺	BNPP	30% DMSO	2.30×10 ⁻⁸	9
[Zn ₃ (L ¹)(X) ₅](CH ₃ OH)(H ₂ O) [Where, X = Cl, Br]	4-PNPP	DMF-H ₂ O (97.5%, v/v)	14.23-17.9	This Work

^aBNPP = bis(4 nitrophenyl)phosphate, 4-PNPP = 4-nitrophenyl-phosphate, HPNP = 2-hydroxypropyl(4-nitrophenyl)phosphate.

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XYZ Coordinates

H₂L

Charge = 0, multiplicity = 1, Nimag = 0, HF = -1647.4594288 a.u.

C	4.779806000	-1.477829000	0.263149000
C	6.096590000	-1.467644000	-0.207391000
C	6.905756000	-0.323900000	-0.210583000
C	6.320394000	0.868870000	0.211259000
C	4.995876000	0.928879000	0.671331000
C	4.221130000	-0.268886000	0.751147000
H	6.505372000	-2.399308000	-0.596311000
H	6.889836000	1.795618000	0.166185000
C	8.346210000	-0.378415000	-0.697818000
H	8.550883000	-1.416738000	-0.992990000
C	8.566230000	0.507058000	-1.938043000
H	9.594308000	0.410890000	-2.307005000
H	7.882033000	0.230452000	-2.747525000
H	8.396099000	1.564776000	-1.702913000

C	9.336242000	-0.011515000	0.422820000
H	9.204252000	-0.661255000	1.294649000
H	10.371801000	-0.106360000	0.074792000
H	9.188540000	1.024005000	0.753078000
O	2.962884000	-0.251322000	1.194002000
H	2.742420000	0.705390000	1.407995000
C	4.361816000	2.226201000	0.888203000
H	4.931709000	3.115218000	0.575189000
C	3.944049000	-2.683186000	0.076157000
H	4.152112000	-3.242987000	-0.854965000
C	2.400591000	3.556862000	1.241515000
H	3.033221000	4.434264000	1.027587000
H	1.869688000	3.729370000	2.183724000
C	1.361872000	3.310120000	0.128539000
H	1.017247000	2.279765000	0.267562000
H	1.876554000	3.323472000	-0.850001000
C	2.057051000	-4.031652000	0.429251000
H	2.249884000	-4.413337000	-0.588924000
H	2.086699000	-4.881335000	1.126074000
C	0.678509000	-3.352590000	0.483540000
H	0.771538000	-2.389861000	-0.033236000
H	0.456545000	-3.111470000	1.539063000
N	3.162748000	2.325448000	1.337011000
N	3.003816000	-3.018938000	0.863653000
N	0.173947000	4.164989000	0.173630000
H	0.385641000	5.075155000	-0.234286000
N	-0.390582000	-4.103469000	-0.179569000
H	-0.473957000	-5.026585000	0.246573000
C	-1.657695000	-3.385392000	-0.029499000
C	-2.755559000	-3.812367000	-1.021266000
H	-2.065644000	-3.423253000	0.996955000
H	-1.451511000	-2.327075000	-0.230705000
H	-3.039693000	-4.859703000	-0.865038000
H	-2.361236000	-3.712666000	-2.044710000
N	-3.912109000	-2.952103000	-0.760786000
C	-3.872785000	-1.806548000	-1.325957000
C	-4.764646000	-0.700878000	-0.934441000
H	-3.087068000	-1.542566000	-2.046416000
C	-5.949063000	-0.905350000	-0.225537000
C	-4.295093000	0.620103000	-1.123151000
C	-6.681301000	0.151030000	0.339120000
H	-6.276212000	-1.932664000	-0.093100000
C	-4.953493000	1.694443000	-0.461665000
O	-3.176113000	0.810885000	-1.839137000
C	-6.141425000	1.431847000	0.243993000

C	-7.981160000	-0.104992000	1.087038000
C	-4.255802000	2.966335000	-0.305740000
H	-2.960629000	1.793179000	-1.778046000
H	-6.637481000	2.260403000	0.747675000
H	-8.358115000	0.868359000	1.431217000
C	-9.050731000	-0.718977000	0.165536000
C	-7.756622000	-0.983787000	2.331437000
H	-4.589861000	3.616312000	0.517242000
N	-3.213814000	3.249899000	-1.003211000
H	-9.996058000	-0.854779000	0.704299000
H	-9.237779000	-0.079555000	-0.704083000
H	-8.732466000	-1.701102000	-0.203919000
H	-7.020133000	-0.532895000	3.005477000
H	-8.693466000	-1.119571000	2.885021000
H	-7.387419000	-1.977123000	2.050688000
C	-2.255365000	4.257965000	-0.576749000
H	-2.474823000	4.659574000	0.424245000
H	-2.242918000	5.092537000	-1.290650000
C	-0.903941000	3.519267000	-0.574689000
H	-0.636473000	3.297602000	-1.625474000
H	-1.080297000	2.548123000	-0.098037000

Int1

Charge = 0, multiplicity = 1, Nimag = 0, HF = -2633.6370152 a.u.

C	-0.212011000	0.347972000	-1.686584000
C	0.579258000	1.514054000	-1.550866000
C	0.013194000	2.755912000	-1.315572000
C	-1.377253000	2.787460000	-1.043477000
C	-2.197949000	1.668973000	-1.130627000
C	-1.658489000	0.439189000	-1.678673000
H	1.661434000	1.439148000	-1.639215000
H	-1.824427000	3.720839000	-0.707032000
C	0.859178000	4.019633000	-1.350799000
H	1.901327000	3.711342000	-1.192954000
C	0.779064000	4.677270000	-2.743409000
H	1.423677000	5.562998000	-2.795524000
H	1.089133000	3.977734000	-3.527085000
H	-0.248697000	4.991226000	-2.963100000
C	0.504027000	5.039671000	-0.256181000
H	0.502457000	4.586278000	0.741521000
H	1.227618000	5.862352000	-0.255217000
H	-0.485471000	5.481696000	-0.422000000
O	-2.383140000	-0.529646000	-2.065921000
C	-3.530174000	1.718661000	-0.541844000
H	-3.893327000	2.713512000	-0.253528000
C	0.267954000	-0.980029000	-1.650136000

H	-0.469445000	-1.763512000	-1.792944000
C	-5.429591000	0.834444000	0.567565000
H	-6.227108000	0.269886000	0.072423000
H	-5.715675000	1.891772000	0.652684000
C	-5.207391000	0.247071000	1.974451000
H	-5.016274000	-0.835343000	1.883437000
H	-6.149301000	0.358083000	2.523040000
C	1.833146000	-2.778708000	-1.072440000
H	1.885522000	-2.894291000	0.013655000
H	1.014292000	-3.411178000	-1.423968000
C	3.175654000	-3.179029000	-1.698109000
H	3.911796000	-2.397014000	-1.483193000
H	3.074670000	-3.230076000	-2.792651000
N	-4.221349000	0.680359000	-0.230900000
N	1.487677000	-1.382042000	-1.369416000
N	-4.140606000	0.947245000	2.700018000
H	-4.393548000	1.012154000	3.683152000
N	3.636665000	-4.439694000	-1.114248000
H	3.463067000	-5.212711000	-1.745888000
C	5.018800000	-4.470925000	-0.633246000
C	5.158904000	-3.858415000	0.773153000
H	5.328655000	-5.520415000	-0.572608000
H	5.721602000	-3.958718000	-1.313181000
H	6.203220000	-3.979530000	1.092922000
H	4.512165000	-4.415839000	1.470494000
N	4.853931000	-2.440288000	0.737337000
C	3.845984000	-2.022720000	1.402305000
C	3.393804000	-0.623008000	1.318500000
H	3.241919000	-2.687253000	2.032887000
C	4.185979000	0.352593000	0.697189000
C	2.124607000	-0.261058000	1.833846000
C	3.790684000	1.692354000	0.598546000
H	5.143424000	0.026838000	0.301132000
C	1.703249000	1.091649000	1.738885000
O	1.347111000	-1.212581000	2.365303000
C	2.551519000	2.034177000	1.140864000
C	4.670567000	2.734147000	-0.076242000
C	0.386756000	1.508165000	2.211260000
H	0.482600000	-0.787621000	2.644607000
H	2.215902000	3.066704000	1.091230000
H	4.156213000	3.701547000	0.011498000
C	6.037115000	2.867289000	0.620133000
C	4.845824000	2.434529000	-1.577042000
H	0.110910000	2.555065000	2.016408000
N	-0.421834000	0.710147000	2.803297000

H	6.633068000	3.661630000	0.155721000
H	5.916717000	3.102601000	1.682986000
H	6.608460000	1.934574000	0.546341000
H	3.878851000	2.402657000	-2.093495000
H	5.460675000	3.203264000	-2.059499000
H	5.340158000	1.467378000	-1.728200000
C	-1.736832000	1.202742000	3.181019000
H	-1.899456000	2.237234000	2.838202000
H	-1.804017000	1.199771000	4.278472000
C	-2.827637000	0.306398000	2.584454000
H	-2.783599000	-0.698079000	3.034858000
H	-2.601941000	0.159962000	1.529153000
Zn	-3.669687000	-1.379934000	-0.718607000
Cl	-5.673121000	-2.295598000	-1.203270000
Cl	-1.977057000	-2.387319000	0.510183000
H	2.185582000	-0.694103000	-1.094062000

TS1

Charge = 0, multiplicity = 1, Nimag = 1 (-163 cm⁻¹), HF = -2633.6357008 a.u.

O	-2.031765000	0.109735000	2.080658000
O	0.751032000	-0.010108000	-2.091802000
N	1.019131000	4.177082000	-0.790344000
N	-2.237511000	-2.686925000	0.029633000
N	-0.129966000	2.170156000	1.290333000
N	-0.222930000	-2.487958000	-2.122849000
N	-3.495950000	-2.171547000	2.119806000
N	3.715155000	2.508414000	-1.014860000
C	2.090249000	-1.976598000	-1.661951000
C	-2.615639000	0.474351000	0.984595000
C	3.339213000	-2.503422000	-1.291278000
H	3.433342000	-3.583064000	-1.186931000
C	0.964029000	-2.875336000	-1.805625000
H	1.169454000	-3.936526000	-1.600683000
C	1.935221000	-0.571765000	-1.779127000
C	4.438186000	-1.692794000	-1.025244000
C	-3.623532000	-0.366723000	0.402789000
C	4.257753000	-0.308807000	-1.142224000
H	5.074909000	0.373204000	-0.926967000
C	-2.297366000	1.676109000	0.267969000
C	-1.138111000	2.506129000	0.561961000
H	-1.132249000	3.464955000	0.034906000
C	-4.121271000	1.277326000	-1.345130000
C	3.040194000	0.265241000	-1.519580000
C	1.031935000	4.365076000	0.669206000
H	0.171170000	4.978613000	0.975737000
H	1.921821000	4.928905000	0.971475000

C	-4.345977000	0.045503000	-0.723020000
H	-5.101727000	-0.626958000	-1.126637000
C	-3.732277000	-1.754428000	0.840142000
H	-4.483476000	-2.346463000	0.312383000
C	-3.079692000	2.054753000	-0.835183000
H	-2.834317000	2.990723000	-1.335777000
C	2.223719000	4.572833000	-1.521343000
H	2.328296000	5.664066000	-1.454288000
H	2.044652000	4.351014000	-2.580714000
C	2.887022000	1.728023000	-1.593379000
H	2.021307000	2.071928000	-2.170369000
C	-4.925702000	1.717108000	-2.558487000
H	-4.551772000	2.706189000	-2.856241000
C	-2.503646000	-2.982273000	-1.382686000
H	-2.868476000	-2.050144000	-1.829720000
H	-3.309146000	-3.724023000	-1.432729000
C	3.566198000	3.954458000	-1.067886000
H	4.365164000	4.345633000	-1.716008000
H	3.814637000	4.319795000	-0.062220000
C	-1.283202000	-3.474625000	-2.169684000
H	-0.954955000	-4.455399000	-1.786305000
H	-1.602902000	-3.618989000	-3.211679000
C	-2.054272000	-3.784485000	0.991294000
H	-1.045310000	-3.719513000	1.401502000
H	-2.188688000	-4.752279000	0.500294000
C	5.771185000	-2.280497000	-0.589125000
H	5.663732000	-3.374344000	-0.592894000
C	1.033824000	3.054862000	1.462079000
H	1.912259000	2.457347000	1.186305000
H	1.115740000	3.245373000	2.539042000
C	-3.123473000	-3.573803000	2.130520000
H	-4.010311000	-4.184415000	1.924059000
H	-2.733023000	-3.856974000	3.109313000
C	6.123697000	-1.850429000	0.847317000
H	6.256713000	-0.763799000	0.908699000
H	7.057893000	-2.322022000	1.175426000
H	5.329045000	-2.127463000	1.547944000
C	6.902970000	-1.919785000	-1.568402000
H	7.065838000	-0.835785000	-1.598468000
H	6.668264000	-2.251346000	-2.586174000
H	7.845153000	-2.389353000	-1.261550000
C	-4.714354000	0.764464000	-3.750692000
H	-5.087246000	-0.241905000	-3.520715000
H	-3.651715000	0.679410000	-4.003870000
H	-5.252539000	1.121276000	-4.636726000

C	-6.422353000	1.864492000	-2.229270000
H	-6.978868000	2.230169000	-3.100353000
H	-6.577433000	2.564927000	-1.401696000
H	-6.857784000	0.900872000	-1.936945000
H	0.088036000	-0.747432000	-2.184629000
H	0.806027000	3.209178000	-1.004398000
H	-1.451049000	-2.029337000	0.128069000
H	-2.846488000	-1.530737000	2.586198000
Zn	-0.056400000	0.372483000	2.434097000
Cl	0.714101000	0.970311000	4.471664000
Cl	0.640087000	-1.564493000	1.334053000

Int2

Charge = 0, multiplicity = 1, Nimag = 0, HF = -2633.6381266 a.u.

O	-1.712477000	-0.976235000	1.208123000
O	0.931130000	0.998190000	-2.202789000
N	1.181976000	3.881597000	0.427482000
N	-2.562939000	-2.403595000	-0.921302000
N	0.219749000	1.154873000	1.474083000
N	-0.178555000	-1.389188000	-2.626530000
N	-3.987879000	-2.707096000	0.964161000
N	3.827798000	3.154421000	-0.530102000
C	2.106327000	-1.095118000	-1.902040000
C	-2.466323000	-0.008205000	0.760125000
C	3.280478000	-1.747224000	-1.487044000
H	3.283289000	-2.834226000	-1.468658000
C	0.960103000	-1.894604000	-2.293369000
H	1.117646000	-2.979547000	-2.302148000
C	2.056152000	0.318851000	-1.886203000
C	4.403141000	-1.050145000	-1.050722000
C	-3.671332000	-0.376902000	0.094464000
C	4.332254000	0.349060000	-1.052313000
H	5.169320000	0.944195000	-0.699850000
C	-2.134769000	1.373230000	0.816247000
C	-0.826697000	1.867174000	1.221728000
H	-0.741704000	2.956637000	1.218784000
C	-4.284520000	1.959312000	-0.240935000
C	3.194956000	1.043645000	-1.474882000
C	1.609191000	3.322353000	1.720027000
H	1.016879000	3.775720000	2.528375000
H	2.662217000	3.552094000	1.933558000
C	-4.548597000	0.586238000	-0.389321000
H	-5.458355000	0.265176000	-0.893970000
C	-3.866564000	-1.839257000	-0.158024000
H	-4.674715000	-2.028974000	-0.874714000
C	-3.070740000	2.314629000	0.344061000

H	-2.812011000	3.370212000	0.414495000
C	2.026688000	4.915378000	-0.153404000
H	1.965421000	5.818519000	0.466646000
H	1.581107000	5.173050000	-1.120665000
C	3.116015000	2.509240000	-1.372785000
H	2.367592000	2.986824000	-2.019495000
C	-5.263659000	3.011285000	-0.739362000
H	-4.819899000	3.993722000	-0.528095000
C	-2.547619000	-2.031187000	-2.361529000
H	-2.782562000	-0.963687000	-2.406898000
H	-3.355390000	-2.590284000	-2.845638000
C	3.552326000	4.574090000	-0.348052000
H	3.929625000	5.162718000	-1.197283000
H	4.122645000	4.899469000	0.528452000
C	-1.219101000	-2.297661000	-3.067320000
H	-0.930318000	-3.354958000	-2.948974000
H	-1.401507000	-2.131524000	-4.138639000
C	-2.518965000	-3.867262000	-0.580186000
H	-1.527766000	-4.077809000	-0.174900000
H	-2.685731000	-4.454378000	-1.486161000
C	5.638497000	-1.777603000	-0.543663000
H	5.467108000	-2.852806000	-0.689670000
C	1.508446000	1.793822000	1.783825000
H	2.236294000	1.358648000	1.088925000
H	1.788215000	1.446453000	2.785618000
C	-3.653925000	-4.044333000	0.474934000
H	-4.538653000	-4.488673000	0.004127000
H	-3.345607000	-4.689015000	1.299791000
C	5.835191000	-1.537469000	0.965297000
H	6.013468000	-0.475073000	1.171596000
H	6.698561000	-2.101287000	1.338271000
H	4.949992000	-1.845715000	1.531587000
C	6.899964000	-1.391923000	-1.336860000
H	7.132608000	-0.327176000	-1.215813000
H	6.771839000	-1.587073000	-2.407604000
H	7.767005000	-1.962735000	-0.984168000
C	-5.476835000	2.918203000	-2.261767000
H	-5.936652000	1.961190000	-2.538785000
H	-4.525641000	3.001594000	-2.799070000
H	-6.141453000	3.716914000	-2.611566000
C	-6.606363000	2.936488000	0.010700000
H	-7.283548000	3.732288000	-0.321824000
H	-6.460554000	3.036935000	1.091529000
H	-7.105919000	1.976587000	-0.170550000
H	0.232687000	0.324654000	-2.430857000

H	1.061497000	3.129540000	-0.244451000
H	-1.778572000	-1.957364000	-0.402158000
H	-3.320816000	-2.405456000	1.674122000
Zn	0.167297000	-0.962159000	1.911790000
Cl	0.799342000	-0.923687000	4.093313000
Cl	0.720709000	-2.877958000	0.670573000

Int3

Charge = 0, multiplicity = 1, Nimag = 0, HF = -3619.8114136 a.u.

O	-1.346885000	2.126624000	-1.101379000
O	1.298732000	-2.151548000	1.993844000
N	1.853287000	-2.631156000	-1.675077000
N	-2.612925000	2.155247000	1.317552000
N	0.723269000	0.293727000	-1.914554000
N	-0.398230000	0.145445000	2.482371000
N	-3.739173000	3.513822000	-0.269846000
N	4.136503000	-3.432741000	-0.547857000
C	1.990252000	0.149798000	1.957163000
C	-2.112744000	1.097865000	-1.374307000
C	3.031932000	1.038198000	1.680224000
H	2.881717000	2.087713000	1.918511000
C	0.766904000	0.700580000	2.521545000
H	0.868564000	1.684873000	2.983562000
C	2.149455000	-1.253100000	1.667385000
C	4.230010000	0.663181000	1.040227000
C	-3.423969000	1.088954000	-0.820085000
C	4.349486000	-0.664135000	0.656251000
H	5.234921000	-0.967723000	0.099780000
C	-1.696640000	-0.049961000	-2.101181000
C	-0.302120000	-0.359903000	-2.350017000
H	-0.151638000	-1.296585000	-2.894115000
C	-3.947314000	-1.030691000	-1.911431000
C	3.343745000	-1.616927000	0.928266000
C	2.309645000	-1.623999000	-2.621092000
H	1.877533000	-1.775914000	-3.626272000
H	3.397039000	-1.741689000	-2.746202000
C	-4.304353000	0.045588000	-1.081943000
H	-5.286407000	0.057141000	-0.613306000
C	-3.743670000	2.159717000	0.174606000
H	-4.663315000	1.940632000	0.730091000
C	-2.642354000	-1.054315000	-2.389186000
H	-2.306302000	-1.930144000	-2.939636000
C	2.159035000	-4.006614000	-1.983636000
H	2.072662000	-4.239449000	-3.056061000
H	1.431769000	-4.626858000	-1.452942000
C	3.259713000	-2.878809000	0.291565000

H	2.425721000	-3.502228000	0.592820000
C	-4.887128000	-2.204766000	-2.134023000
H	-4.421074000	-2.853758000	-2.888056000
C	-2.718107000	1.002603000	2.258522000
H	-2.871518000	0.101172000	1.658309000
H	-3.616516000	1.163485000	2.861391000
C	3.618681000	-4.402369000	-1.517589000
H	3.600150000	-5.402125000	-1.072896000
H	4.320389000	-4.430237000	-2.354700000
C	-1.500540000	0.824341000	3.165916000
H	-1.179370000	1.787443000	3.585959000
H	-1.817200000	0.171433000	3.985133000
C	-2.680919000	3.529580000	1.919881000
H	-1.664352000	3.918427000	1.980593000
H	-3.115062000	3.456080000	2.919572000
C	5.281964000	1.704778000	0.687748000
H	5.000179000	2.635231000	1.197250000
C	2.091773000	-0.188005000	-2.136695000
H	2.614847000	-0.054744000	-1.186445000
H	2.559781000	0.508859000	-2.841650000
C	-3.580999000	4.335715000	0.930953000
H	-4.563353000	4.514867000	1.382228000
H	-3.141133000	5.301401000	0.675727000
C	5.282991000	1.988384000	-0.827694000
H	5.544013000	1.081705000	-1.390425000
H	6.024004000	2.757155000	-1.075225000
H	4.306349000	2.337298000	-1.180071000
C	6.683540000	1.306549000	1.182328000
H	7.043184000	0.400283000	0.678587000
H	6.688609000	1.115061000	2.261099000
H	7.403862000	2.104622000	0.970541000
C	-5.028631000	-3.025729000	-0.836568000
H	-5.509719000	-2.429280000	-0.050841000
H	-4.048062000	-3.338709000	-0.463408000
H	-5.646178000	-3.916464000	-1.004429000
C	-6.259300000	-1.771342000	-2.677376000
H	-6.887836000	-2.647362000	-2.875380000
H	-6.158777000	-1.201184000	-3.607730000
H	-6.794153000	-1.142490000	-1.954840000
H	0.902662000	-2.512535000	-1.324876000
H	-1.733938000	2.113609000	0.762704000
H	-2.946105000	3.637242000	-0.898447000
Zn	0.632954000	2.343762000	-1.241413000
Cl	2.030302000	3.261679000	-2.790618000
Cl	0.709292000	3.426371000	0.854889000

Zn	-0.707463000	-1.945889000	1.933450000
Cl	-1.052497000	-2.874238000	-0.171233000
Cl	-2.275454000	-2.467206000	3.500372000
H	4.885461000	-2.836745000	-0.881384000

TS2

Charge = 0, multiplicity = 1, Nimag = 1 (-211 cm⁻¹), HF = -3619.8019754 a.u.

O	-1.289375000	1.950919000	-0.782785000
O	1.086312000	-2.022233000	0.977399000
N	1.931652000	-2.687987000	-1.694737000
N	-2.540613000	1.996545000	1.544699000
N	0.666576000	0.218017000	-1.896494000
N	-0.317711000	0.030967000	2.483315000
N	-3.710622000	3.426716000	0.050404000
N	4.240611000	-3.354700000	-1.031007000
C	1.999929000	0.108057000	1.686838000
C	-2.116105000	1.002466000	-1.153429000
C	3.104481000	0.967159000	1.591888000
H	3.014667000	1.954618000	2.035569000
C	0.831985000	0.609986000	2.396330000
H	0.976747000	1.575862000	2.887125000
C	2.065439000	-1.177852000	1.054795000
C	4.287356000	0.654721000	0.906936000
C	-3.432383000	1.034925000	-0.617736000
C	4.369448000	-0.611896000	0.327862000
H	5.277705000	-0.905325000	-0.192735000
C	-1.762096000	-0.094883000	-1.983075000
C	-0.388745000	-0.415539000	-2.294543000
H	-0.277118000	-1.325546000	-2.896874000
C	-4.086794000	-0.898305000	-1.957021000
C	3.300650000	-1.513958000	0.402847000
C	2.223428000	-1.665533000	-2.722253000
H	1.657370000	-1.907105000	-3.631323000
H	3.283389000	-1.770339000	-2.988037000
C	-4.383465000	0.108567000	-1.020155000
H	-5.380845000	0.156998000	-0.588381000
C	-3.705210000	2.054698000	0.448025000
H	-4.611382000	1.818664000	1.017733000
C	-2.772084000	-0.991331000	-2.392217000
H	-2.492179000	-1.821583000	-3.038645000
C	2.157068000	-4.062122000	-2.154981000
H	1.903001000	-4.175844000	-3.213187000
H	1.514193000	-4.728034000	-1.575724000
C	3.246940000	-2.792270000	-0.274780000
H	2.633921000	-3.523733000	0.246903000
C	-5.142454000	-1.901815000	-2.392529000

H	-4.660216000	-2.592446000	-3.098185000
C	-2.641711000	0.848723000	2.491026000
H	-2.854462000	-0.045218000	1.893655000
H	-3.490640000	1.044320000	3.153321000
C	3.680894000	-4.401257000	-1.895194000
H	3.756404000	-5.375590000	-1.404333000
H	4.257451000	-4.448524000	-2.821681000
C	-1.361094000	0.636687000	3.304031000
H	-1.027009000	1.575185000	3.769820000
H	-1.589527000	-0.080079000	4.102631000
C	-2.494964000	3.375716000	2.144203000
H	-1.468668000	3.738037000	2.064592000
H	-2.792071000	3.321426000	3.193819000
C	5.355419000	1.729824000	0.754758000
H	5.468522000	2.215292000	1.734880000
C	2.005586000	-0.211645000	-2.299226000
H	2.673946000	0.033948000	-1.474902000
H	2.313056000	0.432271000	-3.132440000
C	-3.487909000	4.199528000	1.272612000
H	-4.440880000	4.321829000	1.800044000
H	-3.098326000	5.191070000	1.035497000
C	4.868215000	2.802619000	-0.244343000
H	4.725153000	2.368002000	-1.241309000
H	5.600513000	3.614201000	-0.329330000
H	3.910085000	3.236571000	0.060453000
C	6.730650000	1.186905000	0.346373000
H	6.711745000	0.776596000	-0.671680000
H	7.078375000	0.400536000	1.026732000
H	7.470383000	1.994161000	0.352443000
C	-5.653170000	-2.735628000	-1.202447000
H	-6.187988000	-2.104514000	-0.481737000
H	-4.824104000	-3.212961000	-0.672037000
H	-6.351885000	-3.507851000	-1.546528000
C	-6.305654000	-1.216046000	-3.132850000
H	-7.036212000	-1.957331000	-3.477735000
H	-5.948500000	-0.652639000	-4.002214000
H	-6.831779000	-0.514565000	-2.473313000
H	1.058726000	-2.535695000	-1.183317000
H	-1.695272000	1.907363000	0.938452000
H	-2.948605000	3.573902000	-0.610372000
Zn	0.639877000	2.281018000	-1.167668000
Cl	1.729448000	3.157823000	-2.972914000
Cl	0.940121000	3.464118000	0.830247000
Zn	-0.615956000	-2.049239000	2.045866000
H	4.832604000	-2.685953000	-1.513195000

Cl	-2.298200000	-2.527182000	0.581404000
Cl	-0.609871000	-2.856686000	4.178849000

Int4

Charge = 0, multiplicity = 1, Nimag = 0, HF = -3619.8041292 a.u.

O	-1.246754000	1.842595000	-0.845626000
O	1.007913000	-1.882494000	0.903702000
N	2.031859000	-2.852800000	-1.381803000
N	-2.551542000	2.100566000	1.445848000
N	0.655361000	0.015853000	-1.899187000
N	-0.366561000	0.175081000	2.438366000
N	-3.619318000	3.466682000	-0.169221000
N	4.310229000	-3.326084000	-0.889995000
C	1.933005000	0.260389000	1.594489000
C	-2.105274000	0.907800000	-1.171349000
C	3.051796000	1.110977000	1.507214000
H	2.965562000	2.103302000	1.940206000
C	0.773121000	0.767345000	2.310379000
H	0.915568000	1.747167000	2.773445000
C	1.995085000	-1.024148000	0.973508000
C	4.236410000	0.772854000	0.851473000
C	-3.428472000	1.025207000	-0.664291000
C	4.312797000	-0.511951000	0.294731000
H	5.230172000	-0.837526000	-0.187898000
C	-1.783811000	-0.244294000	-1.936491000
C	-0.424196000	-0.605236000	-2.253275000
H	-0.347056000	-1.532295000	-2.835851000
C	-4.133751000	-0.968112000	-1.885970000
C	3.227705000	-1.381228000	0.350166000
C	2.173979000	-1.954530000	-2.580443000
H	1.493986000	-2.353471000	-3.337646000
H	3.188481000	-2.099072000	-2.964814000
C	-4.406152000	0.108600000	-1.021340000
H	-5.407289000	0.221530000	-0.610731000
C	-3.683690000	2.126341000	0.322310000
H	-4.613434000	1.967684000	0.880971000
C	-2.820356000	-1.130052000	-2.302099000
H	-2.564230000	-2.004383000	-2.898268000
C	2.232058000	-4.283591000	-1.760683000
H	1.861582000	-4.468350000	-2.769988000
H	1.666365000	-4.899633000	-1.059255000
C	3.194543000	-2.736927000	-0.249073000
H	2.780668000	-3.437607000	0.484191000
C	-5.218139000	-1.963592000	-2.265265000
H	-4.754334000	-2.712401000	-2.922272000
C	-2.682452000	0.995519000	2.438673000

H	-2.910387000	0.080860000	1.879594000
H	-3.528046000	1.236005000	3.090186000
C	3.782498000	-4.501916000	-1.607101000
H	3.966081000	-5.410878000	-1.027421000
H	4.280325000	-4.612630000	-2.573278000
C	-1.403502000	0.794084000	3.256343000
H	-1.066203000	1.740165000	3.704396000
H	-1.630847000	0.093256000	4.069248000
C	-2.504707000	3.502766000	1.986071000
H	-1.464763000	3.831422000	1.973534000
H	-2.888813000	3.503194000	3.008596000
C	5.329965000	1.823252000	0.706398000
H	5.430803000	2.321816000	1.681282000
C	1.959042000	-0.453160000	-2.376711000
H	2.711568000	-0.054709000	-1.700824000
H	2.154389000	0.027141000	-3.343617000
C	-3.399006000	4.316587000	1.002804000
H	-4.363160000	4.543734000	1.471478000
H	-2.929830000	5.257114000	0.709192000
C	4.889061000	2.889374000	-0.320377000
H	4.753639000	2.442785000	-1.312697000
H	5.641380000	3.683138000	-0.401768000
H	3.933958000	3.347249000	-0.042668000
C	6.702807000	1.245533000	0.339191000
H	6.698901000	0.819572000	-0.672467000
H	7.018329000	0.463064000	1.039464000
H	7.458960000	2.037531000	0.350507000
C	-5.759778000	-2.703869000	-1.027879000
H	-6.275805000	-2.011201000	-0.351109000
H	-4.948504000	-3.173861000	-0.464427000
H	-6.482344000	-3.472973000	-1.326555000
C	-6.356075000	-1.291614000	-3.055572000
H	-7.105604000	-2.031710000	-3.359899000
H	-5.977206000	-0.793605000	-3.955130000
H	-6.866197000	-0.535920000	-2.445247000
H	1.169554000	-2.653132000	-0.836977000
H	-1.693699000	1.971811000	0.863165000
H	-2.830842000	3.535121000	-0.811524000
Zn	0.693379000	2.124485000	-1.216320000
Cl	1.917612000	2.833496000	-3.011292000
Cl	0.870130000	3.553100000	0.642619000
Zn	-0.628401000	-1.920824000	2.074042000
H	4.787591000	-2.676173000	-1.508619000
Cl	-2.397391000	-2.486066000	0.747770000
Cl	-0.438890000	-2.688958000	4.212795000

1'

Charge = 0, multiplicity = 1, Nimag = 0, HF = -2698.1689281 a.u.

Zn	0.513765000	-1.488377000	-1.032297000
Zn	-0.513607000	1.491234000	-1.030607000
Cl	0.047803000	2.485512000	-3.007445000
Cl	-0.050238000	-2.478530000	-3.010504000
O	1.247422000	0.383084000	-0.511791000
O	-1.245479000	-0.380421000	-0.508544000
N	-2.537089000	2.389938000	-0.487811000
N	2.537172000	-2.388622000	-0.493299000
N	0.012335000	2.705390000	0.643161000
N	-0.011345000	-2.705798000	0.639328000
N	3.522521000	-1.096996000	-2.035773000
N	-3.521877000	1.100533000	-2.032243000
H	-4.271344000	0.506146000	-2.369008000
C	-2.256704000	-1.827421000	1.115074000
C	2.270219000	0.684838000	0.241899000
C	-3.380986000	-2.111694000	1.922306000
H	-3.337447000	-2.987337000	2.569146000
C	-1.128176000	-2.720011000	1.281244000
H	-1.268942000	-3.483777000	2.059751000
C	-2.269162000	-0.684738000	0.242854000
C	-4.522989000	-1.329623000	1.930256000
C	3.444982000	-0.133146000	0.264601000
C	-4.513462000	-0.203136000	1.088930000
H	-5.388987000	0.444186000	1.070513000
C	2.257437000	1.825190000	1.117178000
C	1.128964000	2.717491000	1.285439000
H	1.269587000	3.478924000	2.066253000
C	4.523046000	1.324677000	1.932707000
C	-3.444283000	0.132631000	0.266395000
C	-2.392992000	2.995677000	0.839649000
H	-2.453001000	2.189643000	1.578373000
H	-3.201011000	3.715286000	1.049386000
C	4.513661000	0.200159000	1.088778000
H	5.388857000	-0.447576000	1.069573000
C	3.600963000	-1.354910000	-0.609923000
H	4.558743000	-1.841378000	-0.315064000
C	3.381264000	2.107092000	1.925882000
H	3.337516000	2.981069000	2.574957000
C	-2.899090000	3.339254000	-1.573365000
H	-2.022345000	3.900165000	-1.898700000
H	-3.670076000	4.037452000	-1.211401000
C	-3.600427000	1.355922000	-0.605893000
H	-4.558424000	1.841532000	-0.310332000

C	5.719950000	1.652424000	2.810666000
H	5.474062000	2.567331000	3.367712000
C	2.393991000	-2.996978000	0.833116000
H	2.454712000	-2.192412000	1.573375000
H	3.202109000	-3.717079000	1.040752000
C	-3.451001000	2.418497000	-2.689778000
H	-4.429977000	2.787631000	-3.031258000
H	-2.766733000	2.372746000	-3.539504000
C	1.025263000	-3.682396000	0.950986000
H	0.960885000	-4.501448000	0.222195000
H	0.904978000	-4.115292000	1.954537000
C	2.898051000	-3.336062000	-1.580867000
H	2.020895000	-3.896116000	-1.906578000
H	3.669093000	-4.035124000	-1.220684000
C	-5.720438000	-1.659746000	2.806619000
H	-5.474745000	-2.576003000	3.361526000
C	-1.024241000	3.681086000	0.957696000
H	-0.960672000	4.501586000	0.230469000
H	-0.903142000	4.112014000	1.961997000
C	3.449452000	-2.413503000	-2.695964000
H	4.427529000	-2.782948000	-3.039623000
H	2.764057000	-2.365250000	-3.544655000
C	-6.978080000	-1.948821000	1.966153000
H	-7.280979000	-1.063220000	1.394065000
H	-7.819877000	-2.233033000	2.608891000
H	-6.797974000	-2.760782000	1.253432000
C	-5.992519000	-0.550365000	3.839608000
H	-6.256059000	0.392641000	3.344916000
H	-5.109944000	-0.365797000	4.462024000
H	-6.826735000	-0.824806000	4.496320000
C	5.991398000	0.540570000	3.841122000
H	6.255529000	-0.401198000	3.344391000
H	5.108397000	0.354328000	4.462442000
H	6.825079000	0.813605000	4.499098000
C	6.978151000	1.943414000	1.971604000
H	7.819442000	2.226604000	2.615456000
H	6.798314000	2.756643000	1.260275000
H	7.281608000	1.058905000	1.398105000
H	4.272652000	-0.502946000	-2.371578000

1

Charge = 0, multiplicity = 1, Nimag = 0, HF = -4145.1346996 a.u.

Zn	-0.324385000	-0.821589000	1.619427000
Zn	-1.210995000	-1.055774000	-1.333999000
Zn	4.916497000	-0.801510000	-0.278557000
Cl	-0.892076000	-3.287129000	-1.519393000

Cl	-0.646664000	-2.898852000	2.474985000
Cl	3.818496000	-0.331992000	-2.283835000
Cl	5.872162000	1.041986000	0.816178000
Cl	5.769574000	-2.864795000	0.218241000
O	0.275491000	-0.215537000	-0.280228000
O	-2.265876000	-0.738552000	0.526761000
N	-3.570101000	-1.100830000	-2.202172000
N	1.552831000	0.032999000	2.425564000
N	-1.238990000	0.467171000	-2.683965000
N	-1.152940000	0.712798000	2.822943000
N	2.979462000	-0.966949000	0.872848000
H	2.343280000	-1.294015000	0.145999000
N	-4.142693000	-2.551679000	-0.573665000
H	-3.206621000	-2.466791000	-0.124799000
H	-4.797083000	-2.898144000	0.132171000
C	-3.328527000	1.072772000	1.755880000
C	0.972274000	0.879315000	-0.586070000
C	-4.477232000	1.879511000	1.877766000
H	-4.477213000	2.646466000	2.650581000
C	-2.271876000	1.329486000	2.727636000
H	-2.498627000	2.128497000	3.446869000
C	-3.286324000	0.061752000	0.741267000
C	-5.608536000	1.746799000	1.078178000
C	2.063754000	1.249533000	0.230909000
C	-5.576338000	0.727495000	0.119792000
H	-6.446511000	0.566509000	-0.514357000
C	0.672634000	1.690600000	-1.725500000
C	-0.387541000	1.452110000	-2.663323000
H	-0.472117000	2.205093000	-3.456469000
C	2.585828000	3.153849000	-1.226662000
C	-4.460613000	-0.091627000	-0.051636000
C	-3.629579000	0.125427000	-3.016940000
H	-3.848912000	0.955010000	-2.339085000
H	-4.435396000	0.066602000	-3.765345000
C	2.833249000	2.359950000	-0.091857000
H	3.712730000	2.557330000	0.512003000
C	2.546348000	0.351311000	1.340953000
H	3.417169000	0.823158000	1.813076000
C	1.502019000	2.809073000	-2.008081000
H	1.288488000	3.391121000	-2.903253000
C	-3.756278000	-2.374569000	-2.932990000
H	-2.838352000	-2.648756000	-3.453773000
H	-4.585637000	-2.298433000	-3.651702000
C	-4.520291000	-1.165485000	-1.088026000
H	-5.557540000	-1.269424000	-1.448884000

C	3.553607000	4.254214000	-1.623761000
H	3.115302000	4.783160000	-2.482549000
C	1.190975000	1.221647000	3.221032000
H	1.152269000	2.074994000	2.535731000
H	1.948478000	1.435335000	3.987763000
C	-4.087811000	-3.402708000	-1.822475000
H	-5.070803000	-3.857659000	-1.954680000
H	-3.314777000	-4.157000000	-1.696288000
C	-0.190270000	1.049535000	3.868160000
H	-0.168212000	0.209065000	4.573423000
H	-0.473068000	1.957224000	4.419150000
C	2.269144000	-1.038518000	3.175673000
H	1.568608000	-1.622189000	3.775985000
H	3.028660000	-0.583964000	3.827123000
C	-6.821216000	2.649435000	1.243689000
H	-6.599261000	3.344733000	2.064199000
C	-2.278346000	0.397845000	-3.699543000
H	-2.041928000	-0.415748000	-4.398460000
H	-2.353417000	1.325146000	-4.283976000
C	2.924538000	-1.876959000	2.056931000
H	3.933382000	-2.204642000	2.312105000
H	2.321215000	-2.753670000	1.813333000
C	-8.076902000	1.849525000	1.637204000
H	-8.362658000	1.146603000	0.844579000
H	-8.926203000	2.521629000	1.803475000
H	-7.909976000	1.273321000	2.553627000
C	-7.075125000	3.488130000	-0.023009000
H	-7.313872000	2.845217000	-0.879671000
H	-6.195955000	4.086081000	-0.286454000
H	-7.921335000	4.168079000	0.126292000
C	3.767531000	5.281275000	-0.498175000
H	4.240409000	4.817296000	0.375070000
H	2.819727000	5.729980000	-0.176194000
H	4.429729000	6.085489000	-0.838463000
C	4.891584000	3.629406000	-2.071615000
H	5.582541000	4.411125000	-2.410645000
H	4.736317000	2.913327000	-2.884572000
H	5.364276000	3.079696000	-1.249641000