The Importance of Tetrel Bonding Interactions with Carbon in Works of Two Arrestive Iso-Structural Cd(II)-Salen Coordination Complexes: A Comprehensive DFT Overview in Crystal Engineering

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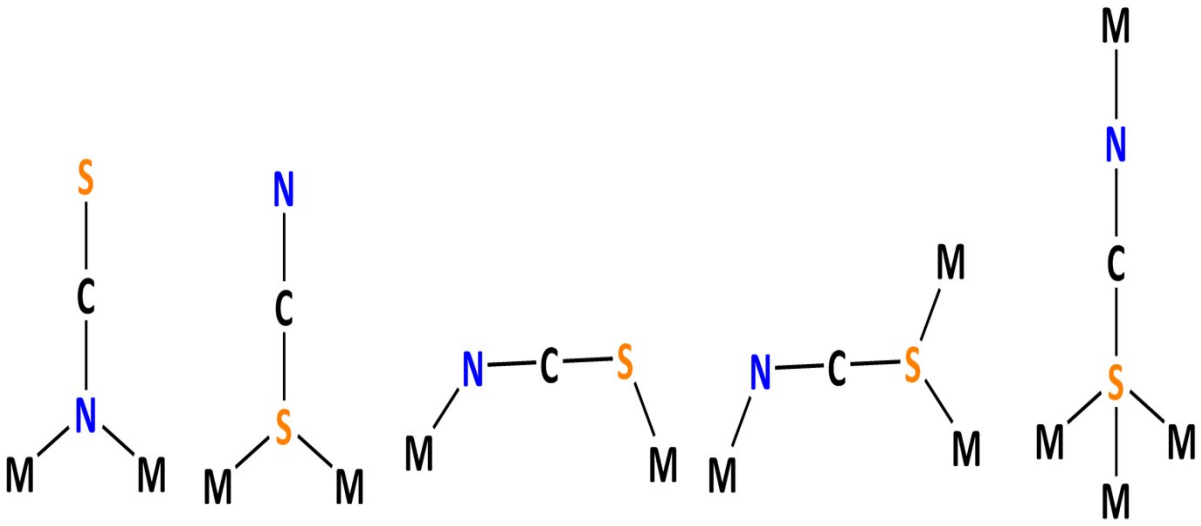
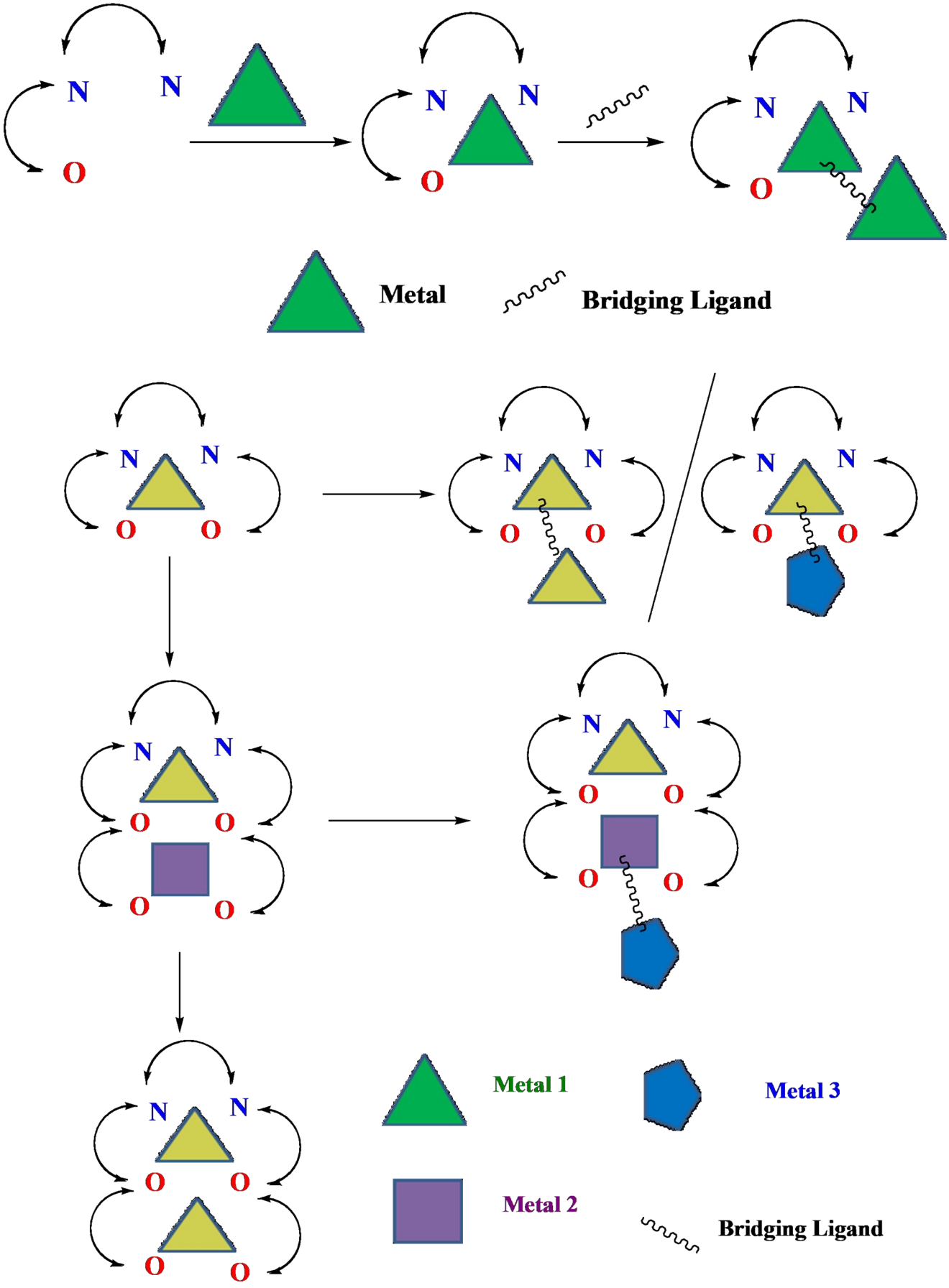
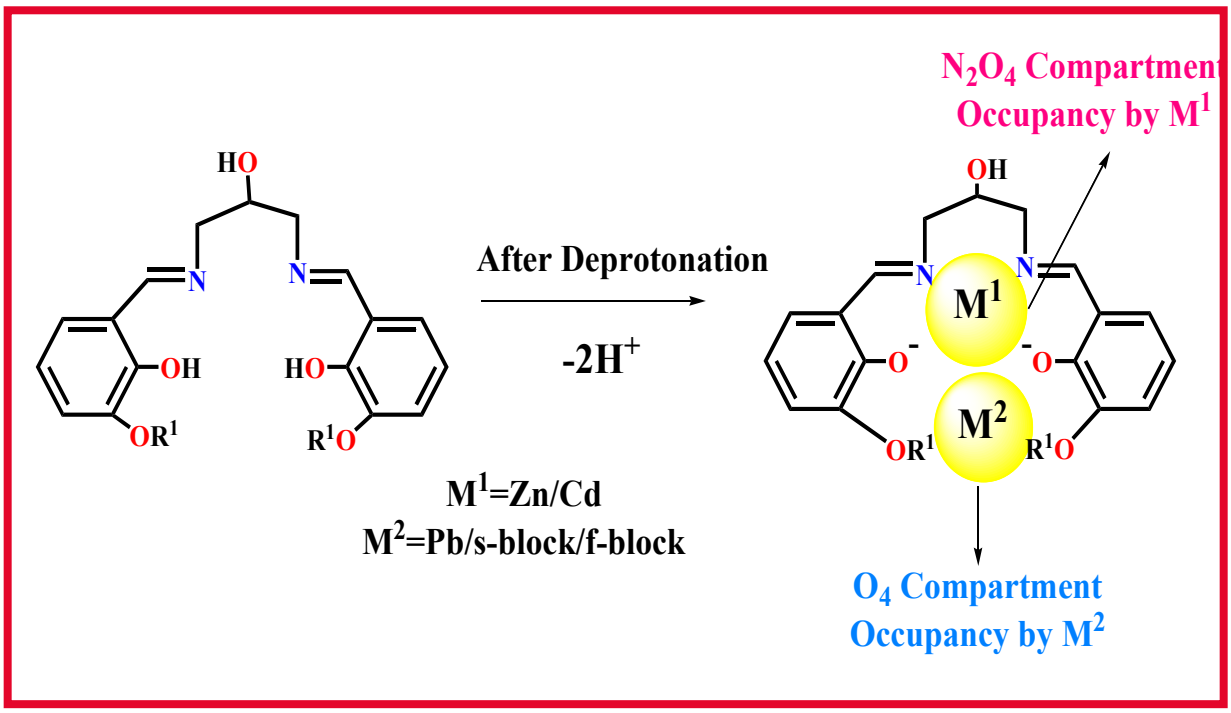


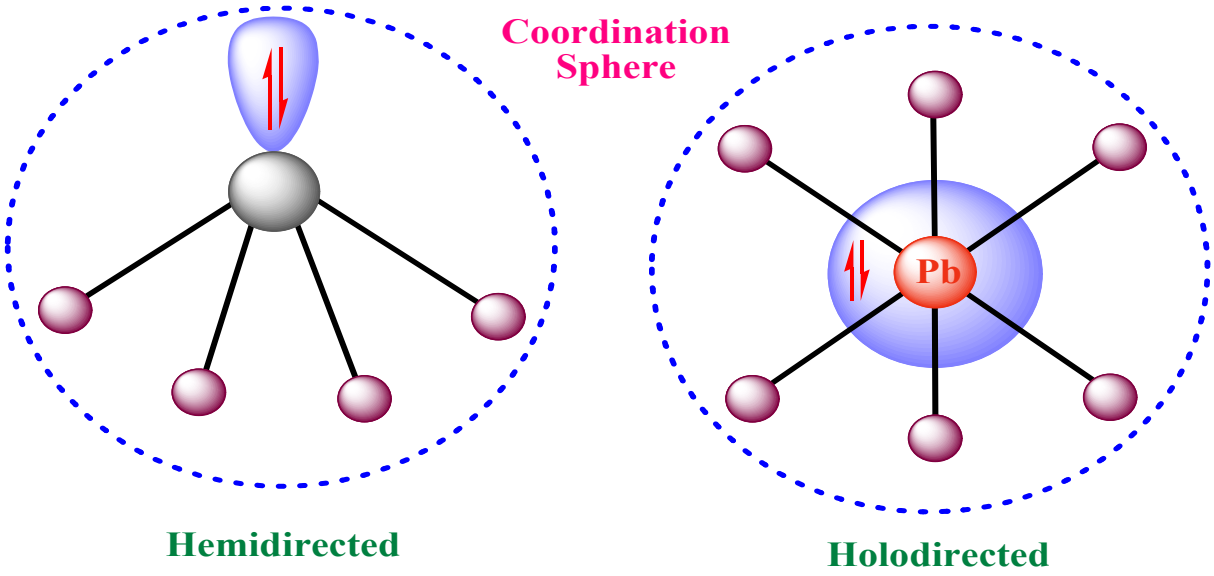
Scheme S1A. Different complexing modes of SCN^- spacer.



SCHEME S1B. Generation of polynuclear complexes in the presence of pseudohalide spacers (SCN^-).



SCHEME S2. Salen ligand compartment mobility (N_2O_2 vs O_4) with M^{2+} metal ion.



SCHEME S3. The simplified Holo-directed and Hemi-directed coordination spheres around.

Table S1 Bond lengths [Å] and angles [°] for complex 1

Cd(1)-O(3)	2.279(6)
Cd(1)-O(6)#1	2.317(8)
Cd(1)-O(2)#1	2.319(6)
Cd(1)-N(2)	2.327(10)
Cd(1)-N(1)	2.352(10)
Cd(1)-O(1)#1	2.440(8)
Cd(1)-O(2)	2.500(6)
Cd(02)-N(3)	2.160(11)
Cd(02)-O(3)	2.223(7)
Cd(02)-O(6)	2.336(9)
Cd(02)-O(2)#1	2.344(6)
Cd(02)-O(5)	2.354(9)
Cd(02)-O(4)	2.382(9)
O(3)-Cd(1)-O(6)#1	92.6(3)
O(3)-Cd(1)-O(2)#1	75.1(2)
O(6)#1-Cd(1)-O(2)#1	105.4(3)
O(3)-Cd(1)-N(2)	78.3(3)
O(6)#1-Cd(1)-N(2)	91.6(4)
O(2)#1-Cd(1)-N(2)	148.8(3)
O(3)-Cd(1)-N(1)	150.8(3)
O(6)#1-Cd(1)-N(1)	87.8(4)
O(2)#1-Cd(1)-N(1)	132.8(3)
N(2)-Cd(1)-N(1)	72.6(4)
O(3)-Cd(1)-O(1)#1	98.4(3)
O(6)#1-Cd(1)-O(1)#1	164.8(3)
O(2)#1-Cd(1)-O(1)#1	67.8(3)
N(2)-Cd(1)-O(1)#1	100.8(4)
N(1)-Cd(1)-O(1)#1	87.7(4)
O(3)-Cd(1)-O(2)	136.0(2)
O(6)#1-Cd(1)-O(2)	73.2(2)
O(2)#1-Cd(1)-O(2)	69.4(3)
N(2)-Cd(1)-O(2)	141.5(3)
N(1)-Cd(1)-O(2)	71.7(3)
O(1)#1-Cd(1)-O(2)	91.6(2)
N(3)-Cd(02)-O(3)	130.4(4)

N(3)-Cd(02)-O(6)	129.9(4)
O(3)-Cd(02)-O(6)	98.5(3)
N(3)-Cd(02)-O(2)#1	103.1(4)
O(3)-Cd(02)-O(2)#1	75.6(2)
O(6)-Cd(02)-O(2)#1	75.9(2)
N(3)-Cd(02)-O(5)	110.4(4)
O(3)-Cd(02)-O(5)	107.8(4)
O(6)-Cd(02)-O(5)	52.3(3)
O(2)#1-Cd(02)-O(5)	128.2(3)
N(3)-Cd(02)-O(4)	89.0(4)
O(3)-Cd(02)-O(4)	68.2(3)
O(6)-Cd(02)-O(4)	124.0(4)
O(2)#1-Cd(02)-O(4)	140.4(3)
O(5)-Cd(02)-O(4)	79.4(4)
Cd(1)#1-O(2)-Cd(02)#1	98.1(2)
Cd(1)#1-O(2)-Cd(1)	100.4(2)
Cd(02)#1-O(2)-Cd(1)	98.6(2)
Cd(02)-O(3)-Cd(1)	103.0(2)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,y,-z+3/2

Table S1 Bond lengths [Å] and angles [°] for complex 2.

Cd(1)-O(3)	2.282(6)
Cd(1)-O(6)#1	2.316(8)
Cd(1)-O(2)#1	2.316(6)
Cd(1)-N(2)	2.329(11)
Cd(1)-N(1)	2.359(10)
Cd(1)-O(1)#1	2.440(8)
Cd(1)-O(2)	2.499(6)
Cd(02)-N(3)	2.166(11)
Cd(02)-O(3)	2.224(7)
Cd(02)-O(6)	2.337(9)
Cd(02)-O(2)#1	2.344(6)
Cd(02)-O(5)	2.356(9)
Cd(02)-O(4)	2.381(9)

O(3)-Cd(1)-O(6)#1	92.5(3)
O(3)-Cd(1)-O(2)#1	75.1(2)
O(6)#1-Cd(1)-O(2)#1	105.3(3)
O(3)-Cd(1)-N(2)	78.2(3)
O(6)#1-Cd(1)-N(2)	91.7(4)
O(2)#1-Cd(1)-N(2)	148.8(3)
O(3)-Cd(1)-N(1)	150.2(3)
O(6)#1-Cd(1)-N(1)	87.7(4)
O(2)#1-Cd(1)-N(1)	133.4(3)
N(2)-Cd(1)-N(1)	72.0(4)
O(3)-Cd(1)-O(1)#1	98.3(3)
O(6)#1-Cd(1)-O(1)#1	164.8(3)
O(2)#1-Cd(1)-O(1)#1	67.6(3)
N(2)-Cd(1)-O(1)#1	100.9(4)
N(1)-Cd(1)-O(1)#1	88.2(4)
O(3)-Cd(1)-O(2)	136.0(2)
O(6)#1-Cd(1)-O(2)	73.2(3)
O(2)#1-Cd(1)-O(2)	69.4(3)
N(2)-Cd(1)-O(2)	141.6(3)
N(1)-Cd(1)-O(2)	72.3(3)
O(1)#1-Cd(1)-O(2)	91.6(2)
N(3)-Cd(02)-O(3)	130.3(4)
N(3)-Cd(02)-O(6)	130.0(4)
O(3)-Cd(02)-O(6)	98.5(3)
N(3)-Cd(02)-O(2)#1	103.2(4)
O(3)-Cd(02)-O(2)#1	75.6(2)
O(6)-Cd(02)-O(2)#1	75.8(2)
N(3)-Cd(02)-O(5)	110.4(5)
O(3)-Cd(02)-O(5)	107.8(4)
O(6)-Cd(02)-O(5)	52.4(3)
O(2)#1-Cd(02)-O(5)	128.1(3)
N(3)-Cd(02)-O(4)	89.1(4)
O(3)-Cd(02)-O(4)	67.9(3)
O(6)-Cd(02)-O(4)	124.0(4)
O(2)#1-Cd(02)-O(4)	140.3(3)
O(5)-Cd(02)-O(4)	79.4(4)
Cd(1)#1-O(2)-Cd(02)#1	98.2(2)
Cd(1)#1-O(2)-Cd(1)	100.5(2)

Cd(02)#1-O(2)-Cd(1)	98.7(2)
Cd(02)-O(3)-Cd(1)	102.9(2)
Cd(1)#1-O(6)-Cd(02)	104.3(3)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,y,-z+3/2

TABLE S2 Reported Covalent, and Tetrel bond lengths (Å) distances for Pb(II) complexes.

Complexes	Bond lengths (Å)	Bond Nature	Ref
$[PbL]ClO_4]_n .nH_2O$	Pb-N 2.408(4)-2.513(4)	Covalent	1
	2.934(4)	**Tetrel**	
	Pb-O 2.382(4)	Covalent	
	ClO_4^- 3.201(5)	**Tetrel**	
{[Pb(HL)(OAc)]ClO_4}*n*	Pb-N 2.612(6)-2.755(7)	Covalent	1
	Pb-O 2.572(5)-2.515(6)	Covalent	
	ClO_4^- 3.047(7)	**Tetrel**	
	ClO_4^- 3.309(10)	**Tetrel**	
[PbL(NO_2)]*n*	Pb-N 2.452(4)-2.837(3)	Covalent	1
	3.436(4)	**Tetrel**	
	Pb-O 2.384(5)-2.904(5)	Covalent	
	3.299(4)	**Tetrel**	
[PbLN_3]*n*	Pb-N 2.571(3)-2.837(3)	Covalent	1
	3.436(4)	**Tetral**	
	N_3^- 2,321(3)-2.883(3)	Covalent	
	Pb-O 2.335(3)	Covalent	
[$Pb_2(HL)_2(NO_3)_2(NCS)_2$]	Pb-N 2.663(3)-2.460(4)	Covalent	1
	Pb-O 2.555(2)-2.882(2)	Covalent	
	Pb-S NCS^- 3.2246(11)	**Tetrel**	
[PbL(OAc)]$_2$	Pb-N 2.490(3)-2.613(4)	Covalent	1
	3.030(4)-3.489(3)	**Tetrel**	
	Pb-O 2.383(3)-2.753(4)	Covalent	
		This work	

TABLE S3 EDX analysis of weight (%) contribution of elements

Complex	% C		% O		% Cd		% S		% Na	
	Calcd	**Obsd**	**Calcd**	**Obsd**	**Calcd**	**Obsd**	**Calcd**	**Obsd**	**Cald**	**Obsd**
1	41.6	42	17.41	17.88	25.8	26.02	8.77	8.81	5.31	5.29

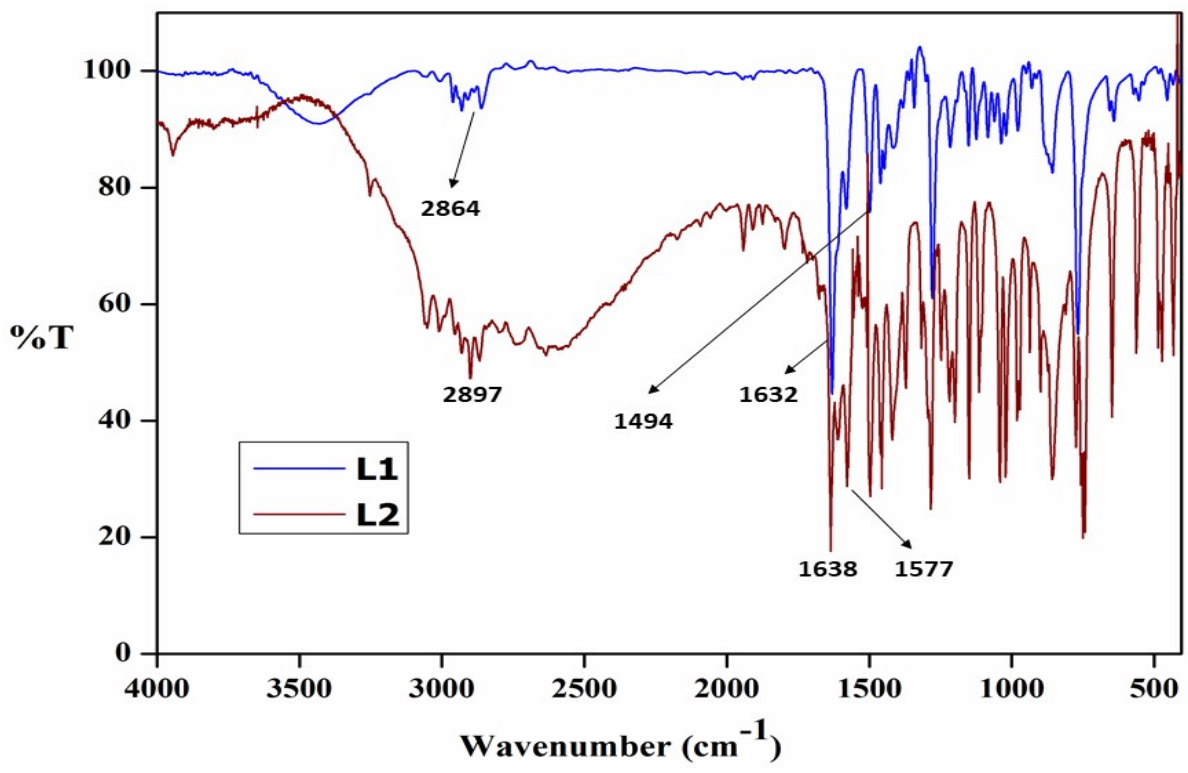


Fig.S1. Representative IR spectra for Salen ligands.

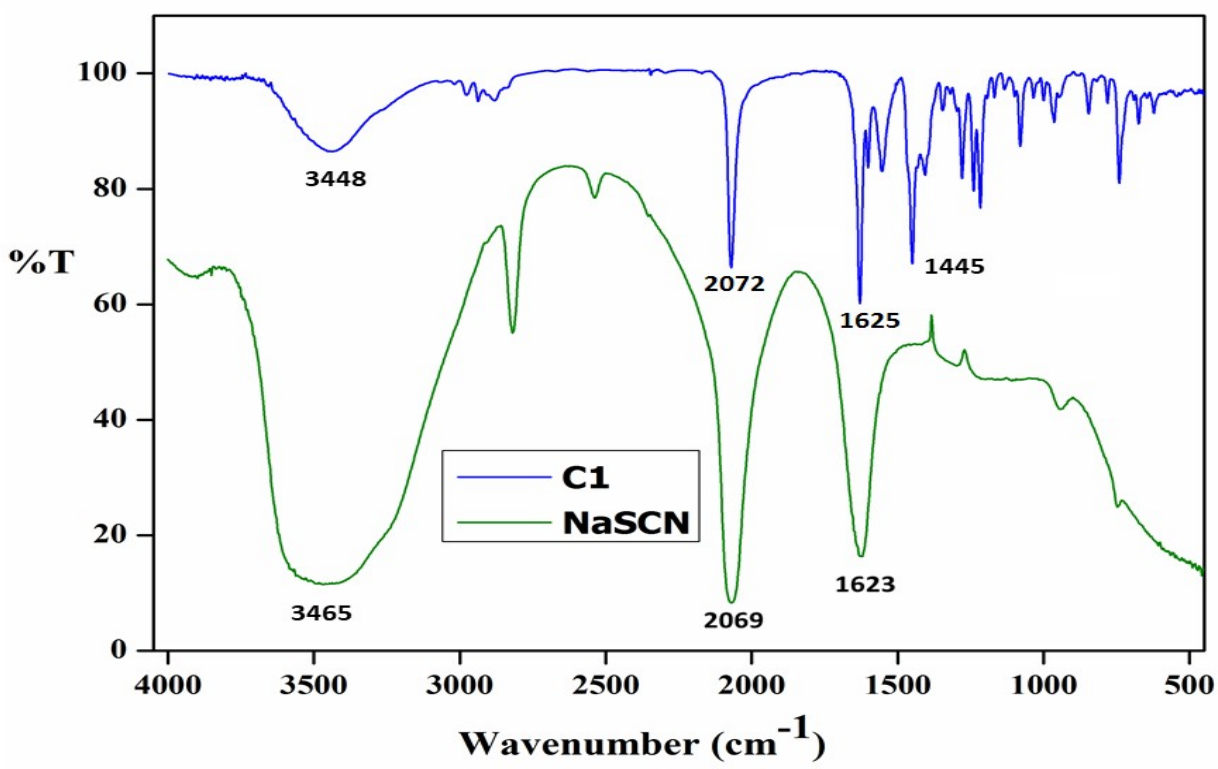


Fig.S2. Representative IR spectra for **1**.

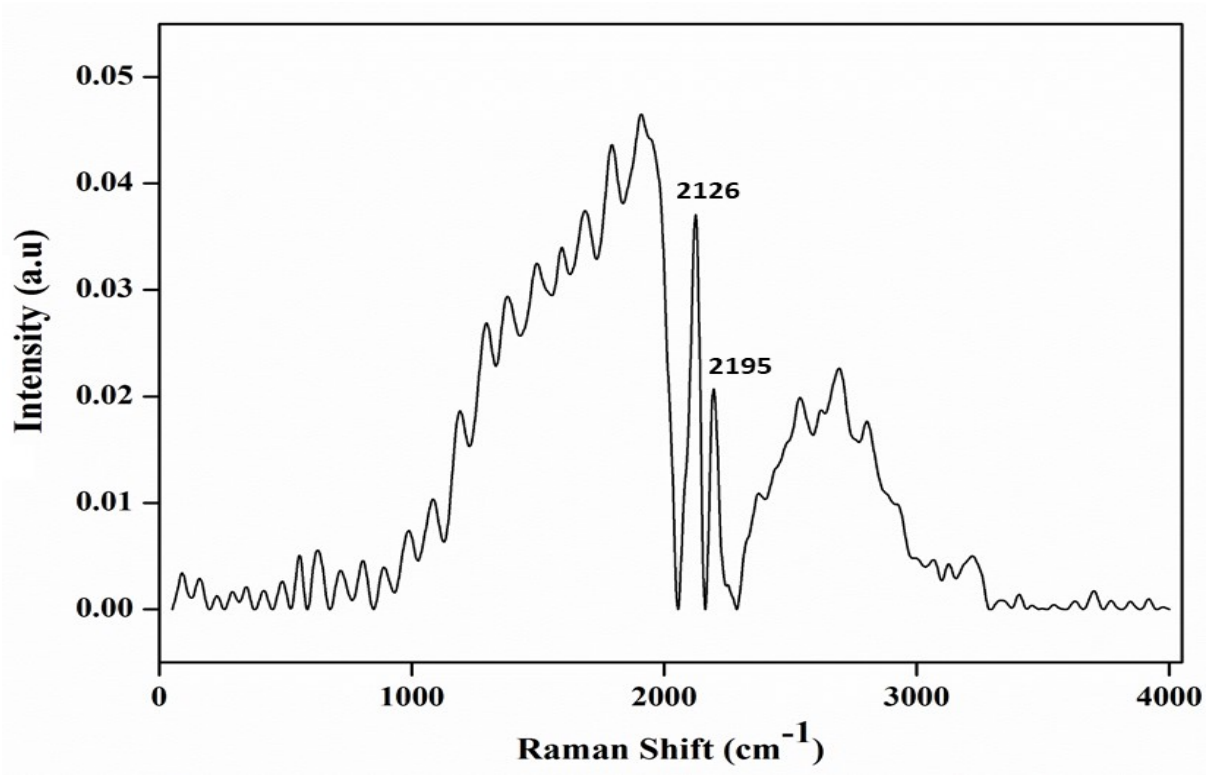


Fig.S3. Representative Raman spectra for **1**.

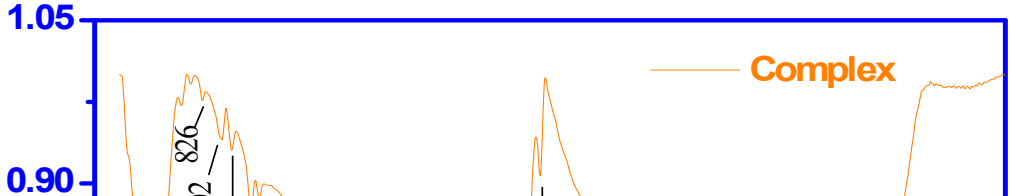


Fig.S2. Representative IR spectra for **2**.

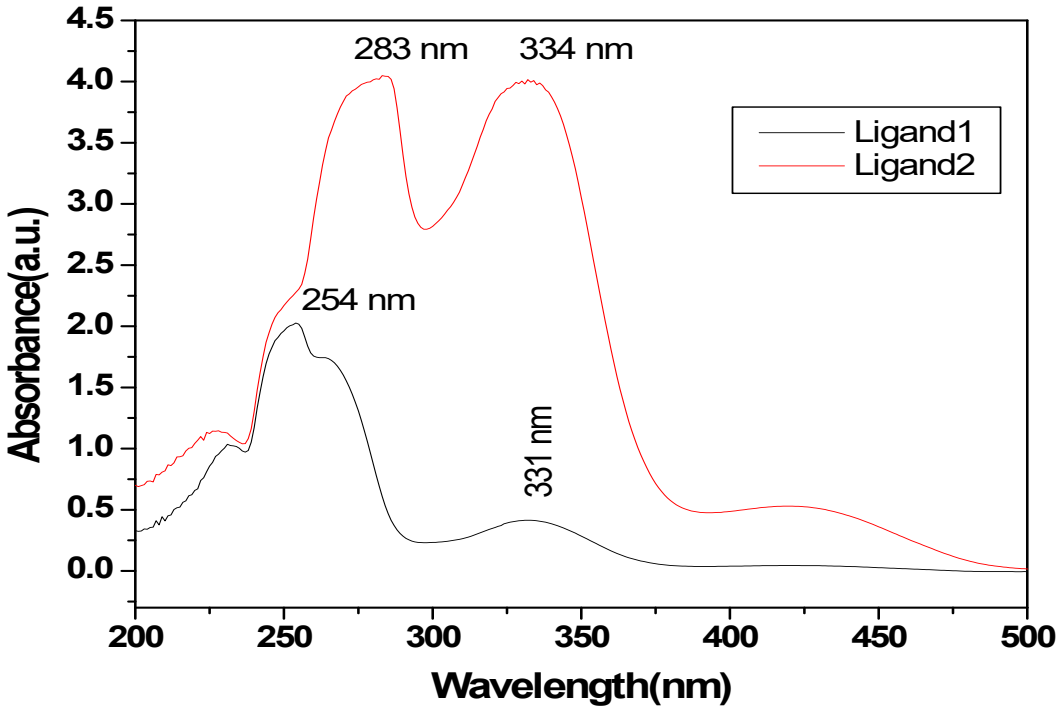


Fig.S4. Representative UV-Vis for the Salen ligands.

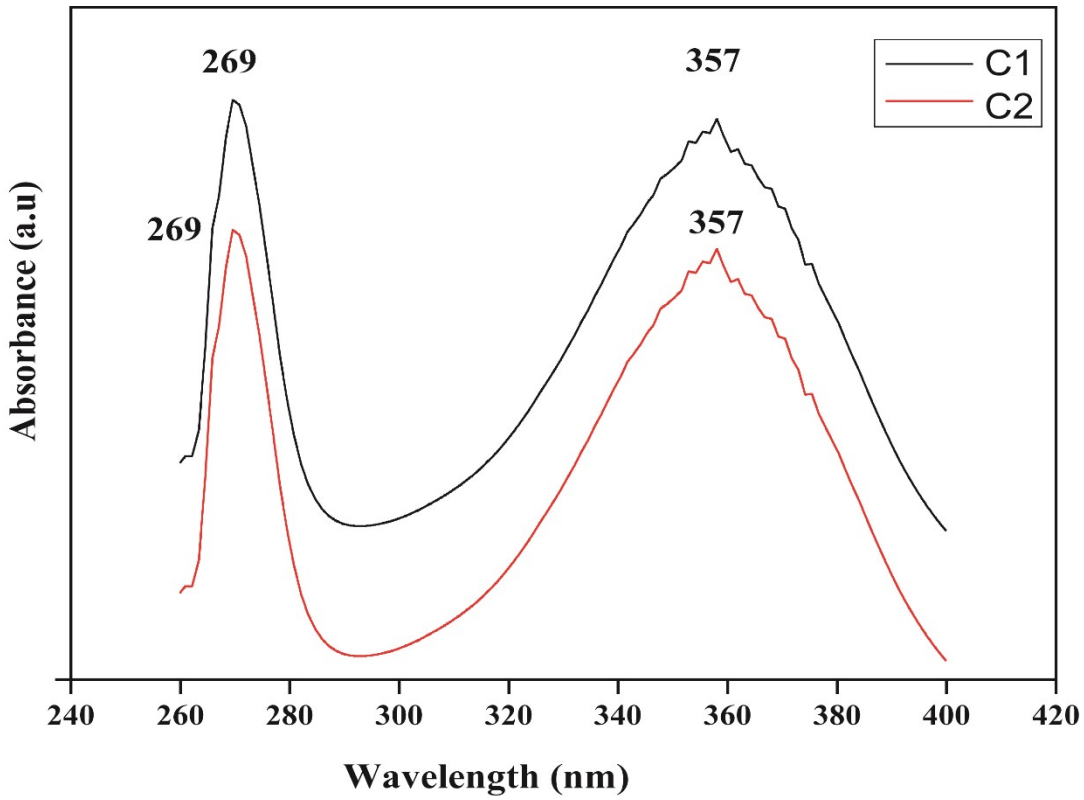


Fig.S5. Representative UV-Vis for the complexes.

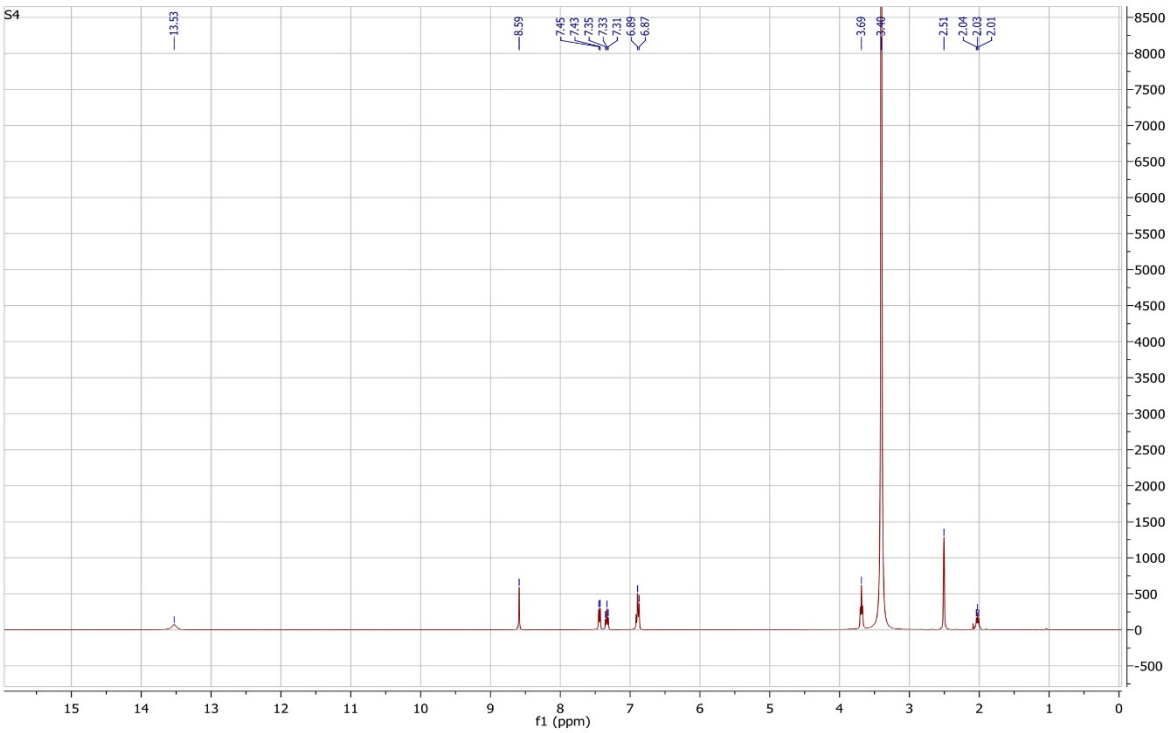


Fig.S6. Representative ^{1}H NMR spectra for H_2L^1.

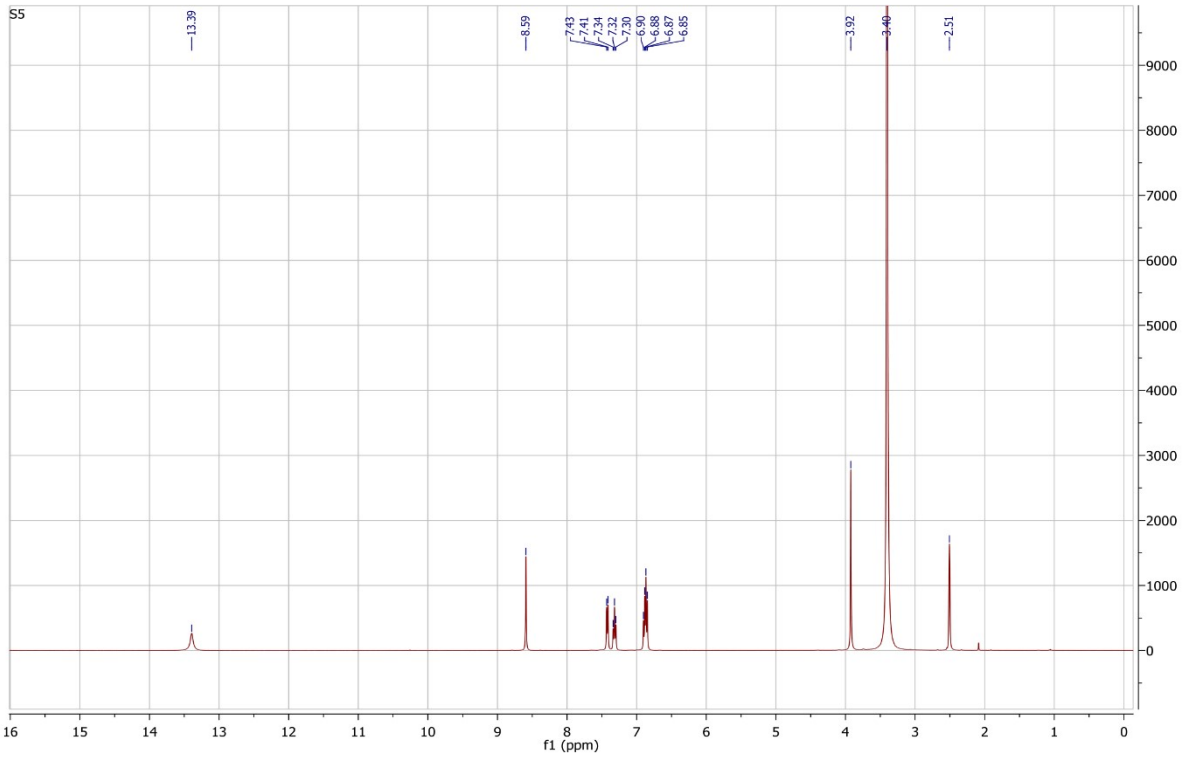


Fig.S6. Representative ^{1}H NMR spectra for H_2L^2.

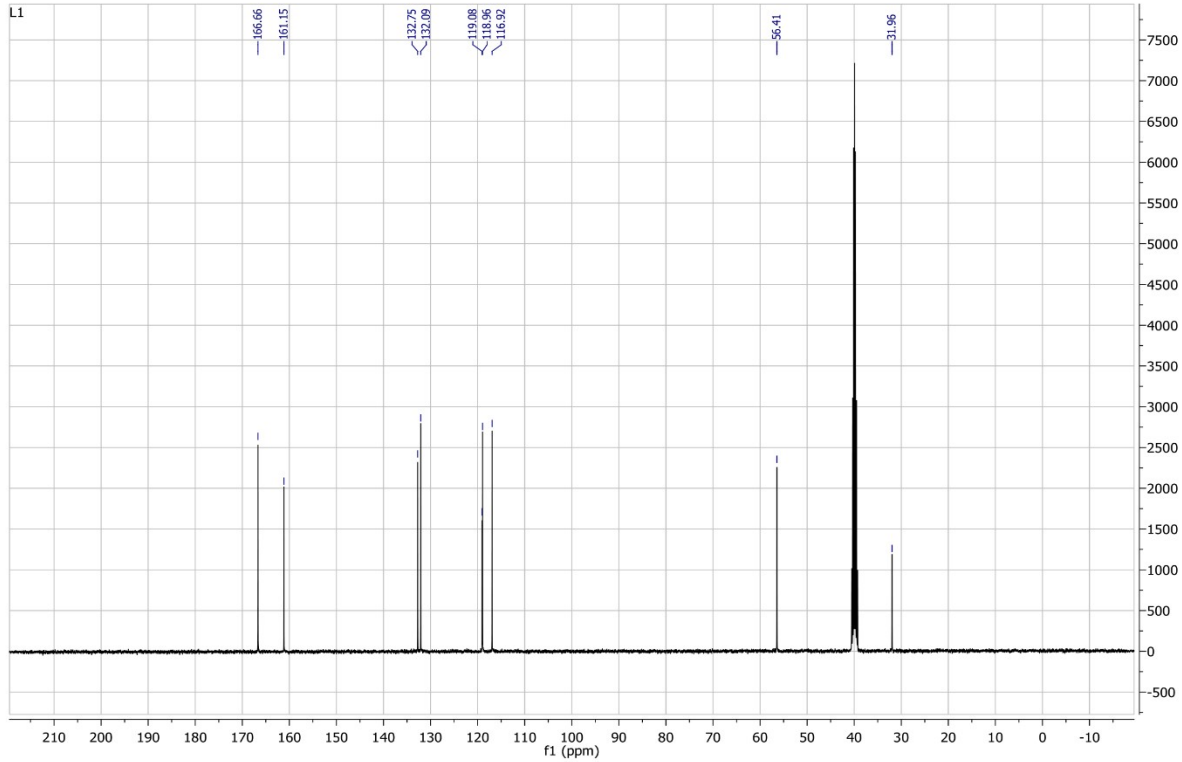


Fig.S7. Representative ^{13}C NMR spectra for H_2L^1.

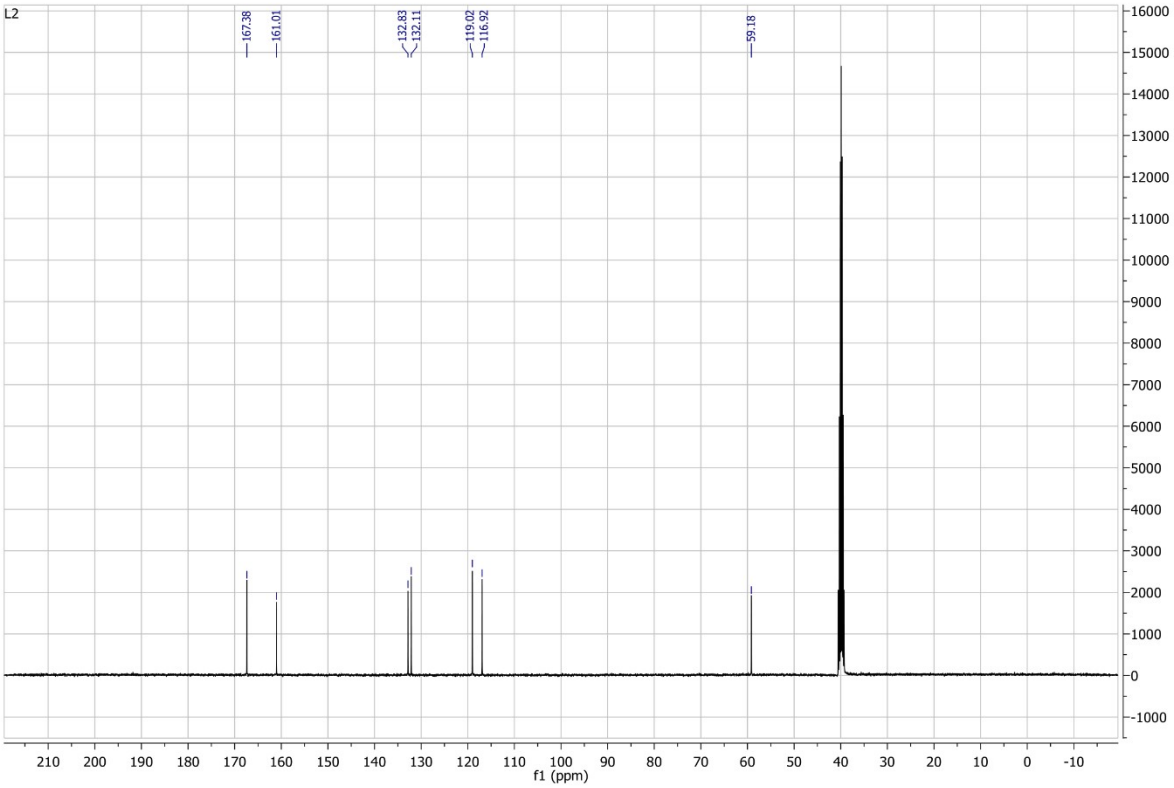


Fig.S7. Representative ^{13}C NMR spectra for H_2L^2.

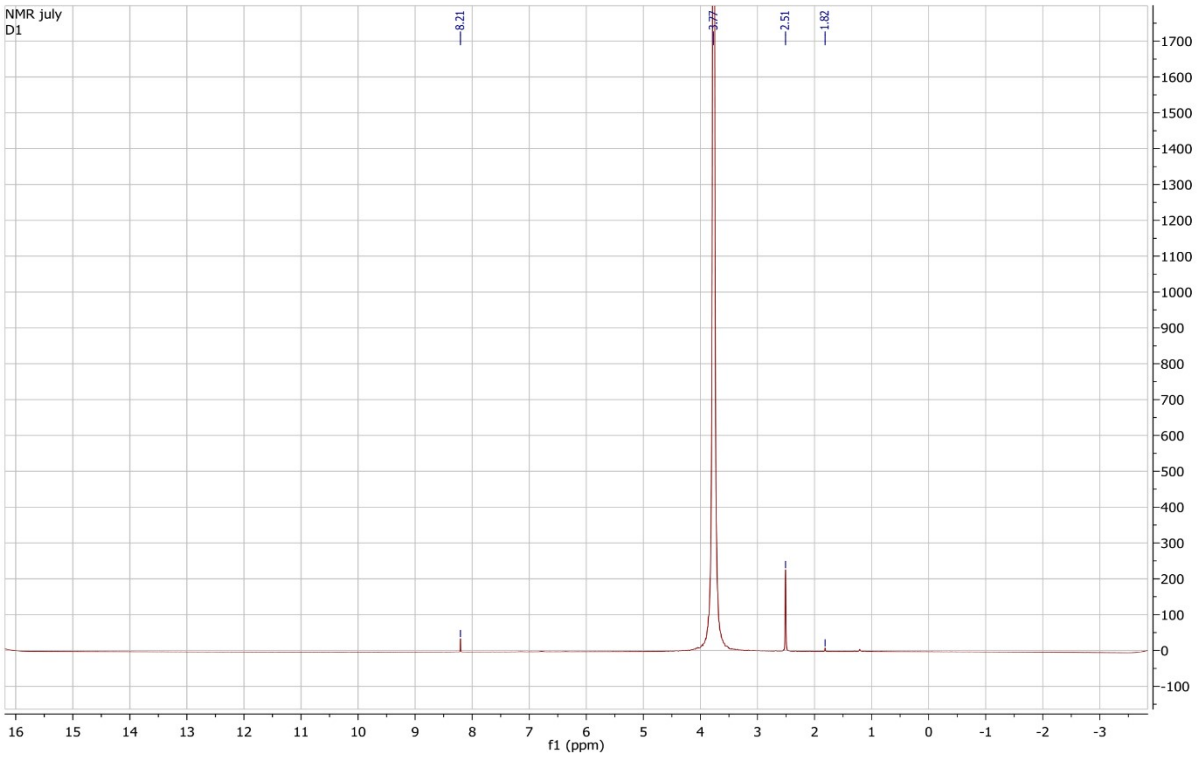


Fig.S8. Representative ^{1}H NMR spectra for **1**.

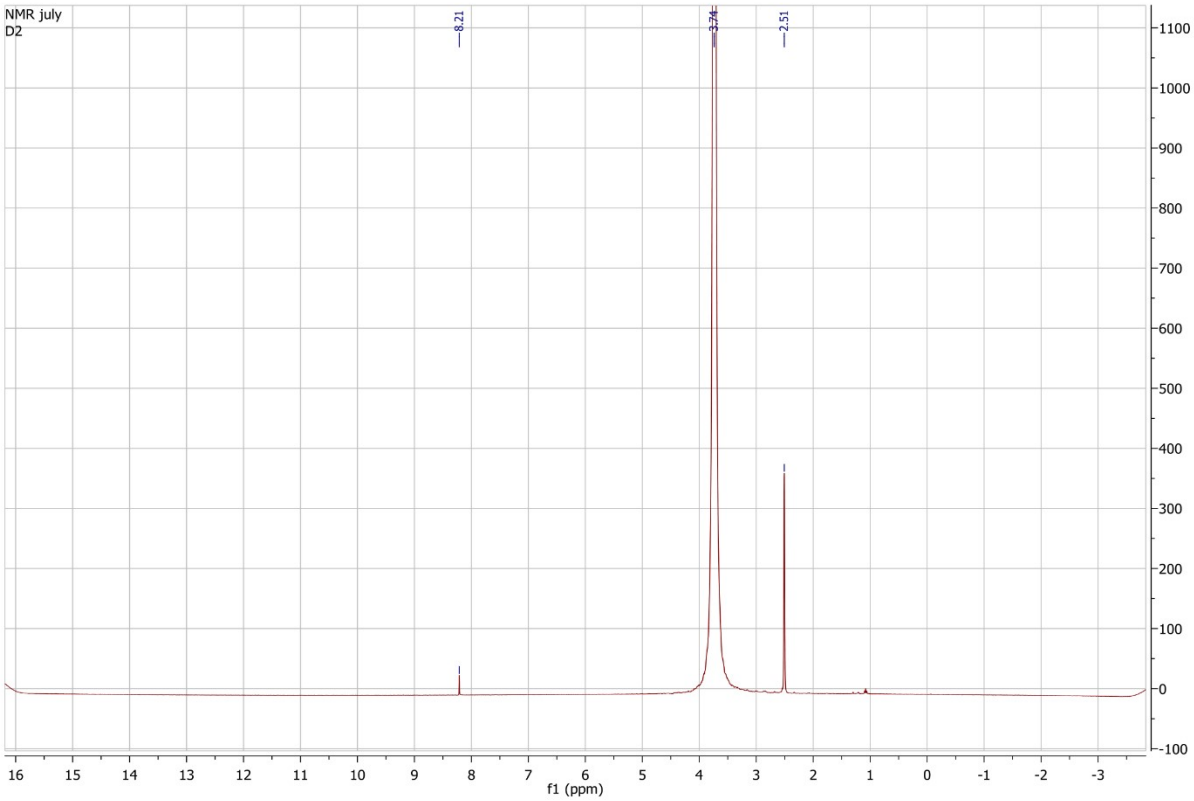


Fig.S8. Representative ^{1}H NMR spectra for **2**.

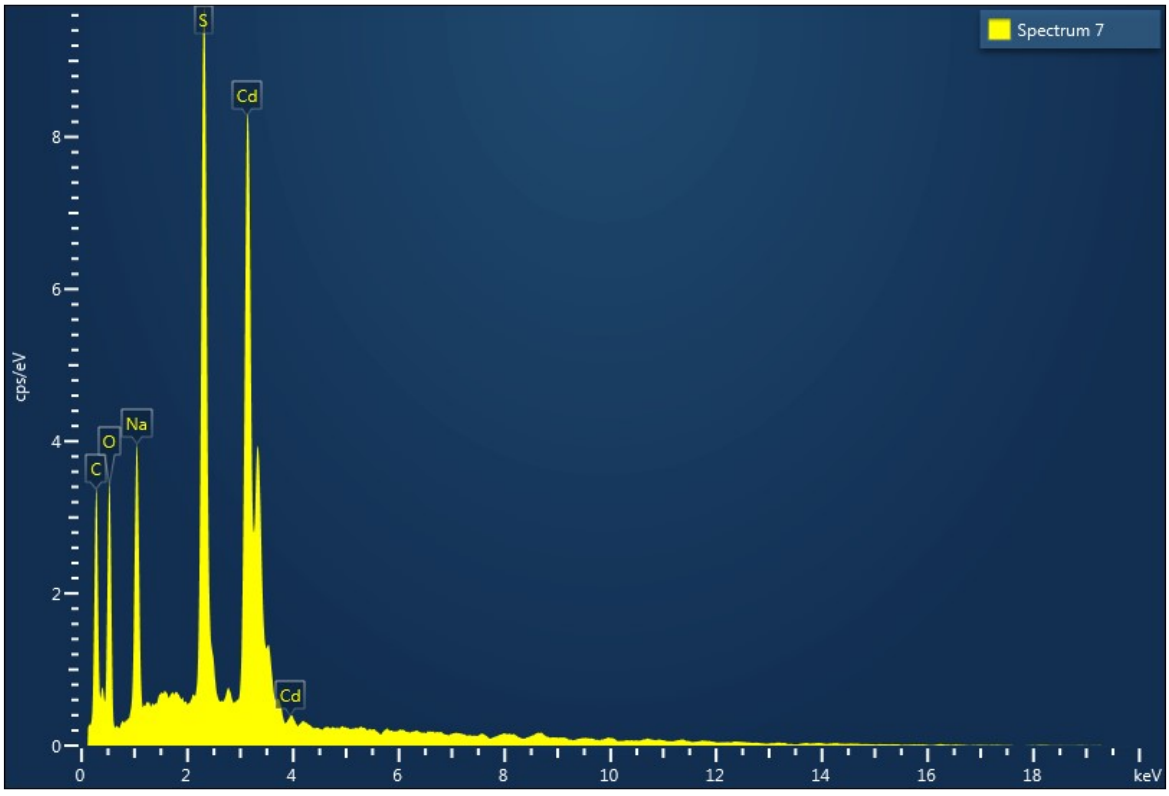
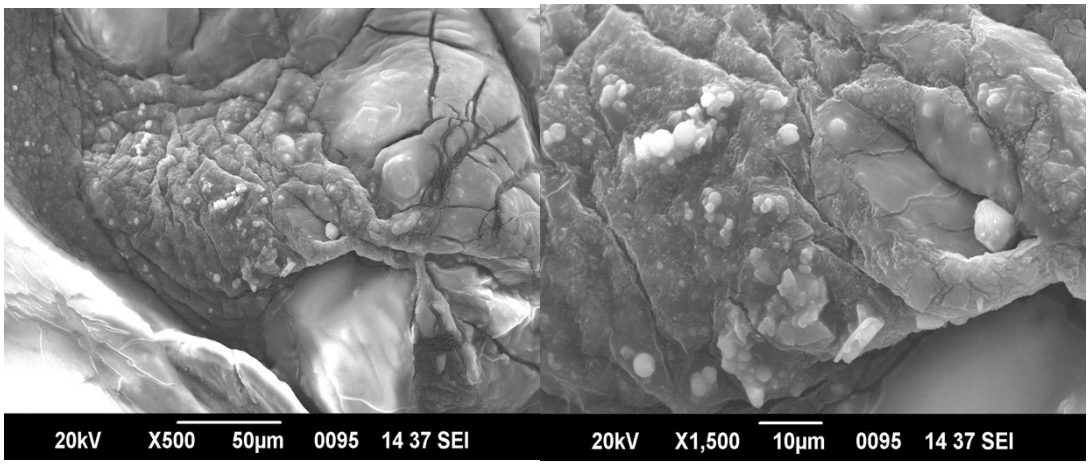
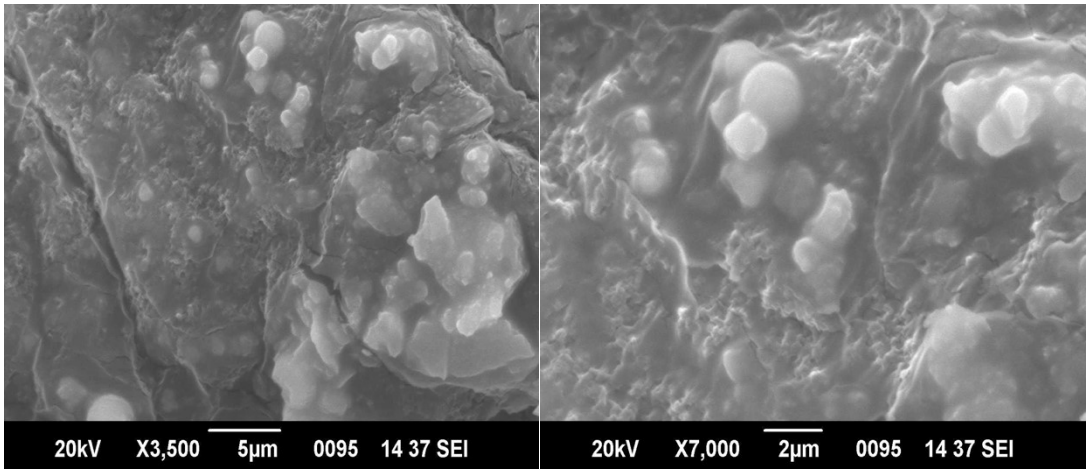


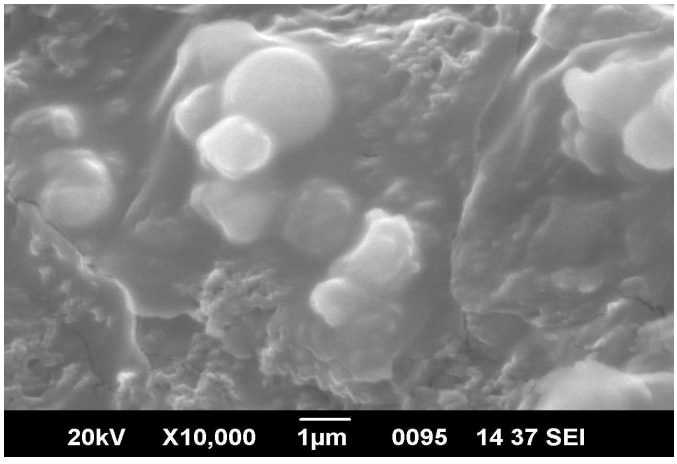
Fig.S9. EDX profile for **1**.



(a) **(b)**



(c) **(d)**



(e) **Fig.S10.** SEM image profile for **1 (a-e)**

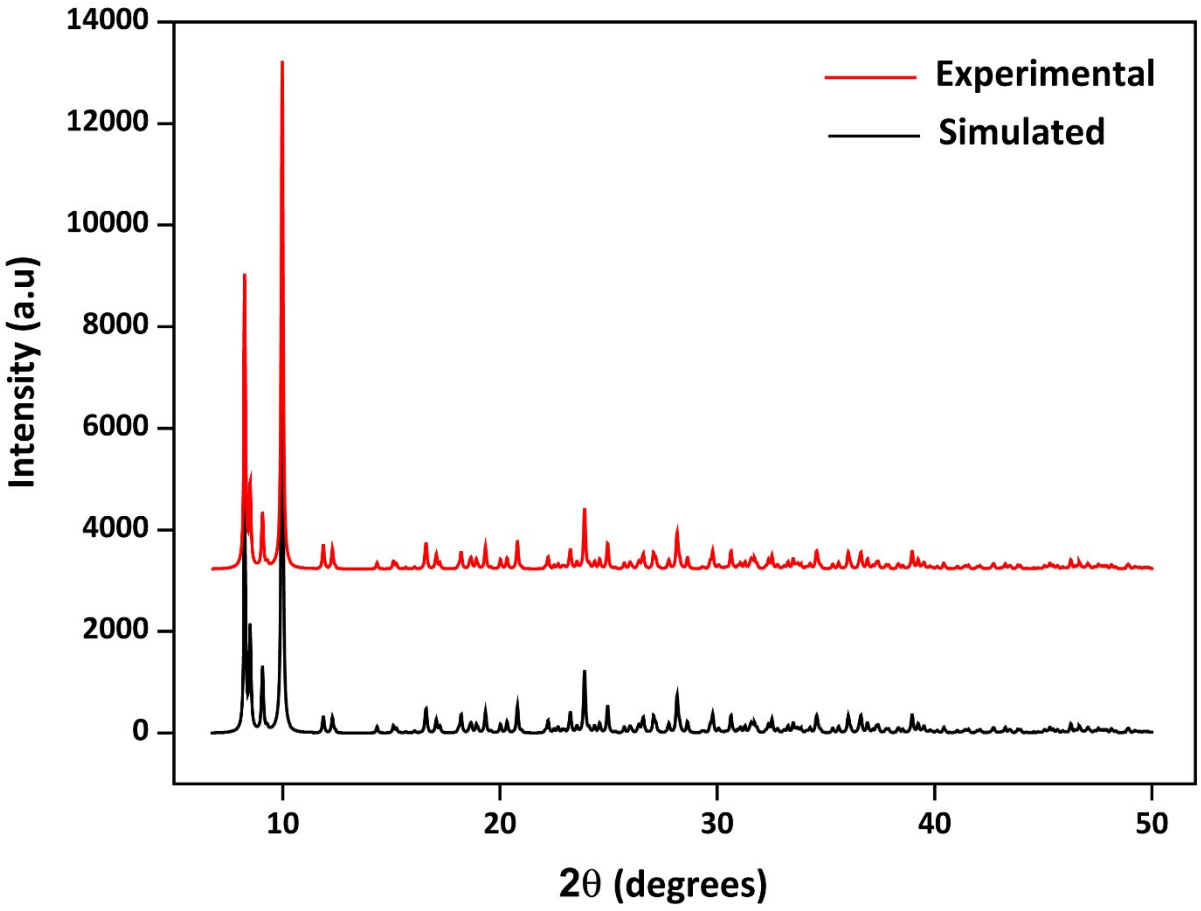


Fig.S11. PXRD profile for **1**.

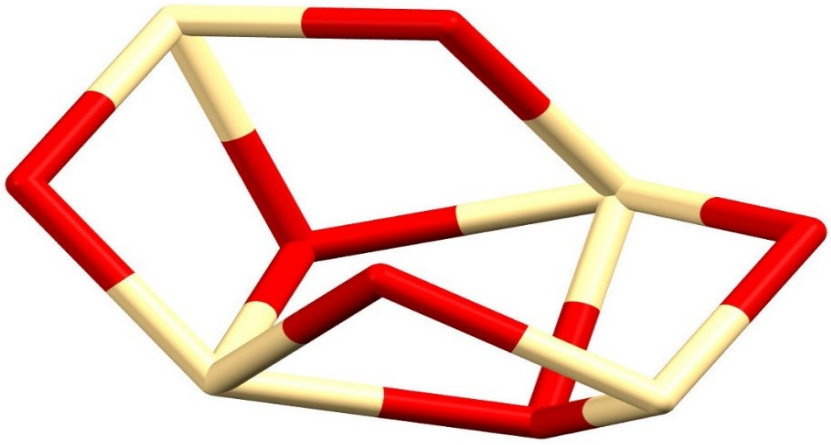


Fig.S12. An unusual open cubane structure was observed in the complexes.

References

1 G. Mahmoudi, D. A. Safin, M. P. Mitoraj, M. Amini, M. Kubicki, T. Doert, F. Locherer, and M. Fleck, *Inorg. Chem. Front.*, 2017, **4,** 171–182.