Electronic Supplementary Information

Non-covalent tetrel bonding interactions in hemidirectional lead(II) complexes with nickel(II)-salen type metalloligands

Sourav Roy,[a] Michael G. B. Drew,[b] Antonio Bauzá,[c] Antonio Frontera[c] and Shouvik Chattopadhyay*[a]

[a]Department of Chemistry, Inorganic Section, Jadavpur University, Kolkata - 700032, India.

Tel: +9133-2457-2941; E-mail:shouvik.chem@gmail.com

[b]School of Chemistry, The University of Reading, P.O. Box 224, Whiteknights, Reading RG6 6AD, United Kingdom,

[c]Department of Chemistry, Universitat de les Illes Balears, Crta de Valldemossa km 7.5, 07122 Palma de Mallorca (Baleares), SPAIN; E-mail:toni.frontera@uib.es

---

Table S1: Selected bond angles (°) for complexes **1**-**4**.

Complex	1	2	3	4
O(11)-Ni(1)-N(19)	90.86(15)	90.9(3)	91.0(2)	91.4(4)
O(11)-Pb(1)-O(131)	62.13(11)	64.7(2)	61.34(17)	64.2(3)
N(19)-Ni(1)-N(23)	97.43(16)	-	97.7(3)	95.0(5)
O(11)-Ni(1)-N(23)	169.57(16)	-	171.3(2)	169.9(4)
O(11)-Ni(1)-O(31)	79.83(15)	-	80.9(2)	82.3(4)

O(31)-Ni(1)-N(19)	170.59(16)	-	171.7(2)	172.5(5)
O(11)-Pb(1)-O(31)	66.96(12)	-	69.16(19)	71.0(3)
O(11)-Pb(1)-O(291)	127.66(11)	-	118.63(18)	131.1(3)
O(31)-Pb(1)-O(291)	63.22(12)	-	61.10(17)	63.0(3)
O(31)-Pb(1)-O(131)	128.85(12)	-	128.23(18)	133.2(4)
O(131)-Pb(1)-O(291)	157.79(11)	-	133.98(17)	147.6(3)
N(1)-Ni(1)-N(23)	91.56(18)	-	89.3(3)	92.8(5)
O(31)-Ni(1)-N(23)	91.68(16)	-	90.4(2)	90.7(4)
O(11)-Ni(1)-N(1)	94.92(16)	-	91.6(3)	94.6(5)
N(1)-Ni(1)-N(19)	88.93(18)	-	87.9(3)	93.0(5)
O(31)-Ni(1)-N(1)	93.20(17)	-	94.3(3)	91.6(5)
O(1)-Ni(1)-O(11)	-	92.1(3)	90.6(2)	82.9(4)
O(1)-Ni(1)-N(19)	-	91.0(4)	87.8(3)	88.7(5)
Cl(1)-Pb(1)-O(11)	-	85.77(19)	-	88.3(3)
Cl(1)-Pb(1)-O(131)	-	99.11(16)	-	78.3(2)
O(1)-Ni(1)-O(31)	-	-	90.3(2)	86.4(4)
O(1)-Ni(1)-N(1)	-	-	175.2(3)	177.0(5)
O(1)-Ni(1)-N(23)	-	-	89.2(2)	89.5(4)
Cl(1)-Pb(1)-Cl(1[a])	-	165.21(7)	-	-
Cl(1)-Pb(1)-O(11[a])	-	82.02(18)	-	-

Cl(1)-Pb(1)-O(131[a])	-	83.20(16)	_	-
O(11[a])-Pb(1)-O(131[a])	-	64.7(2)	_	_
O(1)-Ni(1)-O(1[a])	-	178.6(3)	_	_
O(1)-Ni(1)-O(11[a])	-	86.9(3)	-	_
O(1)-Ni(1)-N(19[a])	-	90.0(4)	-	_
Cl(1[a])-Pb(1)-O(11)	-	82.02(18)	-	_
O(11)-Pb(1)-O(11[a])	-	68.6(3)	-	-
O(11)-Pb(1)-O(131[a])	-	133.0(2)	-	-
Cl(1[a])-Pb(1)-O(131)	-	83.20(16)	-	-
O(1[a])-Ni(1)-O(11)	-	86.9(3)	-	-
O(11)-Ni(1)-O(11[a])	-	79.6(3)	-	-
O(11[a])-Pb(1)-O(131)	-	133.0(2)	_	-
O(131)-Pb(1)-O(131[a])	-	162.2(2)	_	-
O(11)-Ni(1)-N(19[a])	_	170.2(3)	_	-
O(1[a])-Ni(1)-N(19)	_	90.0(4)	_	_
O(11[a])-Ni(1)-N(19)	_	170.2(3)	_	_
N(19)-Ni(1)-N(19[a])	_	98.7(4)	_	_
O(1[a])-Ni(1)-O(11[a])	_	92.1(3)	_	_
O(1[a])-Ni(1)-N(19[a])	_	91.0(4)	_	_
O(11[a])-Ni(1)-N(19[a])	_	90.9(3)	_	_

Cl(1[a])-Pb(1)-O(11[a])	-	85.77(19)	-	-
Cl(1[a])-Pb(1)-O(131[a])	-	99.11(16)	-	-
O(3)-Pb(1)-O(11)	-	-	77.2(2)	-
O(3)-Pb(1)-O(31)	-	-	90.2(2)	-
O(3)-Pb(1)-O(131)	-	-	92.86(18)	-
O(3)-Pb(1)-O(291)	-	-	133.09(18)	-
S(1[b])-Pb(1)-O(3)	-	-	78.32(14)	-
S(1[b])-Pb(1)-O(11)	-	-	147.61(14)	-
S(1[b])-Pb(1)-O(31)	-	-	90.11(15)	-
S(1[b])-Pb(1)-O(131)	-	-	140.99(12)	-
S(1[b])-Pb(1)-O(291)	-	-	66.44(13)	-
O(1)-Pb(1)-O(2)	50.45(16)	-	-	-
O(1)-Pb(1)-O(11)	124.25(15)	-	-	-
O(1)-Pb(1)-O(31)	87.10(15)	-	-	-
O(1)-Pb(1)-O(131)	125.62(14)	-	-	-
O(1)-Pb(1)-O(291)	68.43(14)	-	-	-
O(2)-Pb(1)-O(11)	78.52(13)	-	-	-
O(2)-Pb(1)-O(31)	86.97(14)	-	-	-
O(2)-Pb(1)-O(131)	87.67(14)	-	-	-
O(2)-Pb(1)-O(291)	113.05(13)	-	-	-

O(1W)-Ni(1)-O(11)	86.75(14)	-	-	-
O(1W)-Ni(1)-O(31)	89.90(15)	-	-	-
O(1W)-Ni(1)-N(1)	176.70(16)	-	-	-
O(1W)-Ni(1)-N(19)	88.20(16)	-	-	-
O(1W)-Ni(1)-N(23)	87.20(16)	-	-	-
Cl(1)-Pb(1)-O(31)	-	-	-	87.7(3)
Cl(1)-Pb(1)-O(291)	-	-	-	74.4(2)

Symmetry transformations: [a] = -x,y,1/2-z; [b] = 1/2-x,1/2+y,1/2-z.

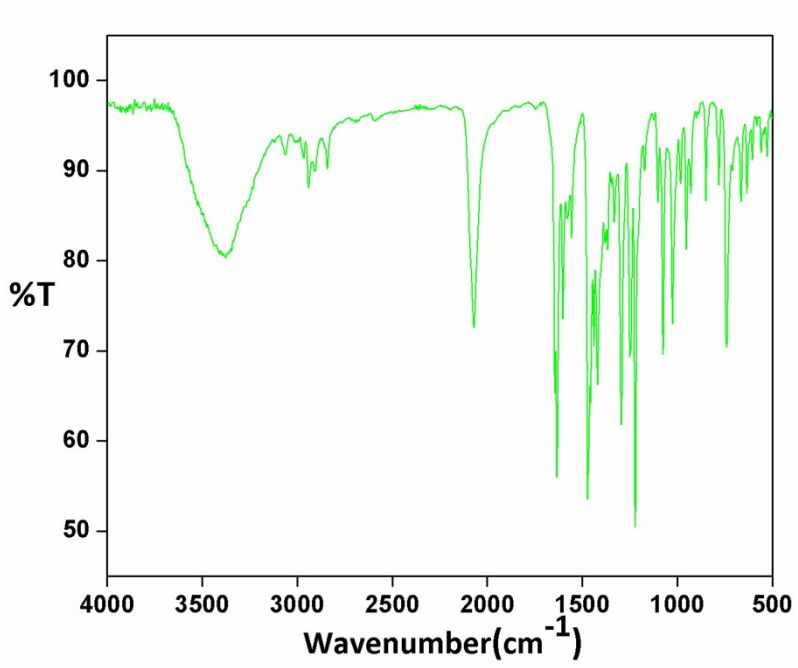

Fig. S1: IR spectrum of complex **1**.

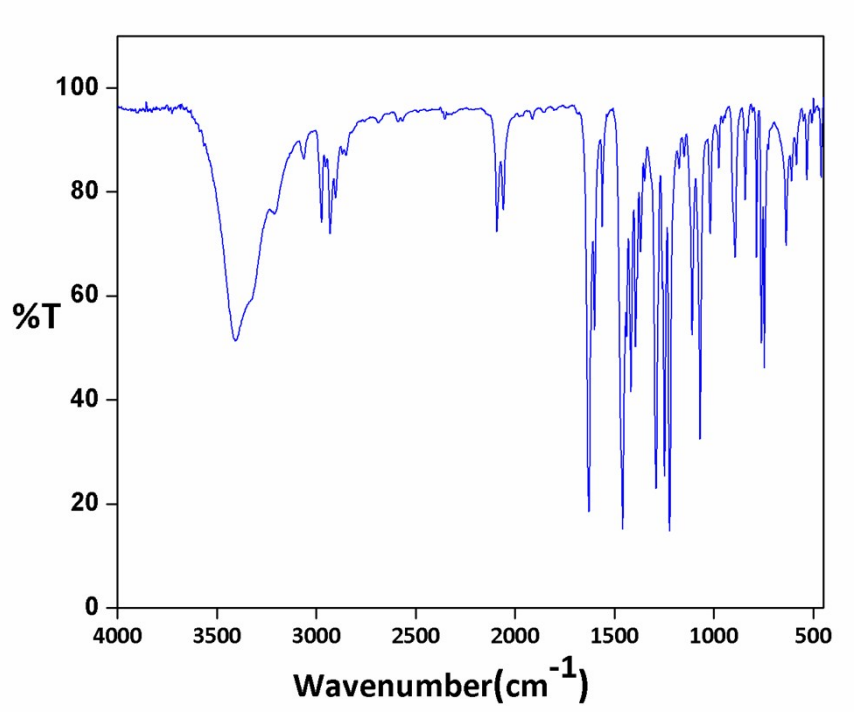

Fig. S2: IR spectrum of complex **2**.

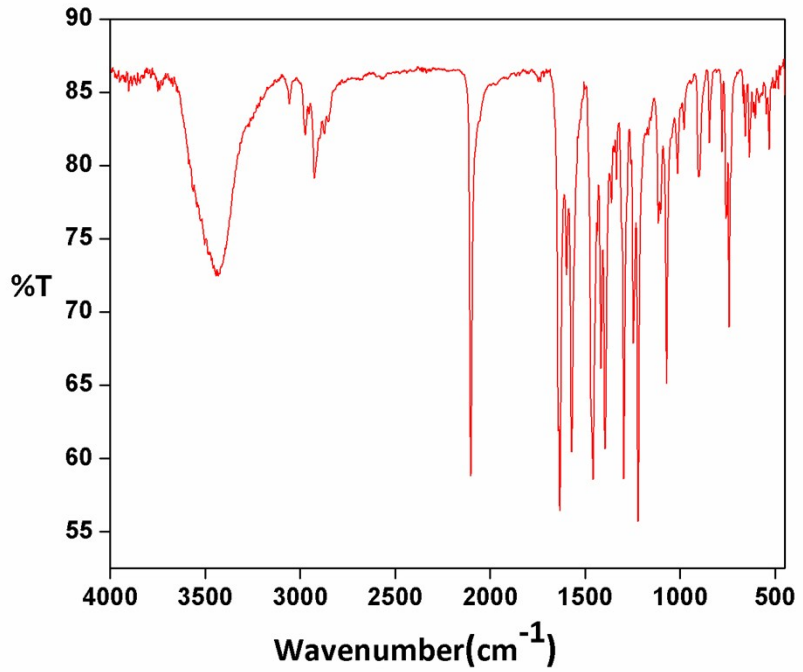

Fig. S3: IR spectrum of complex **3**.

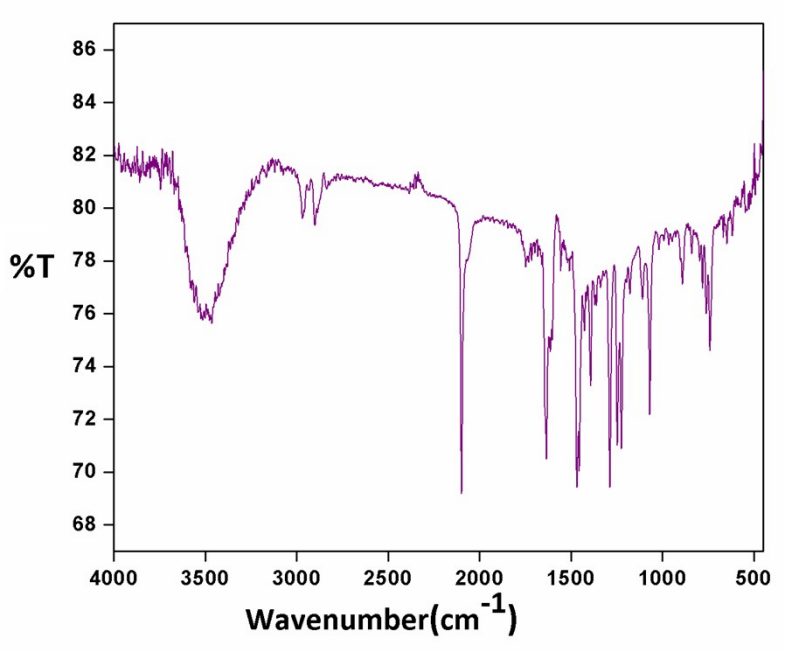

Fig. S4: IR spectrum of complex **4**.

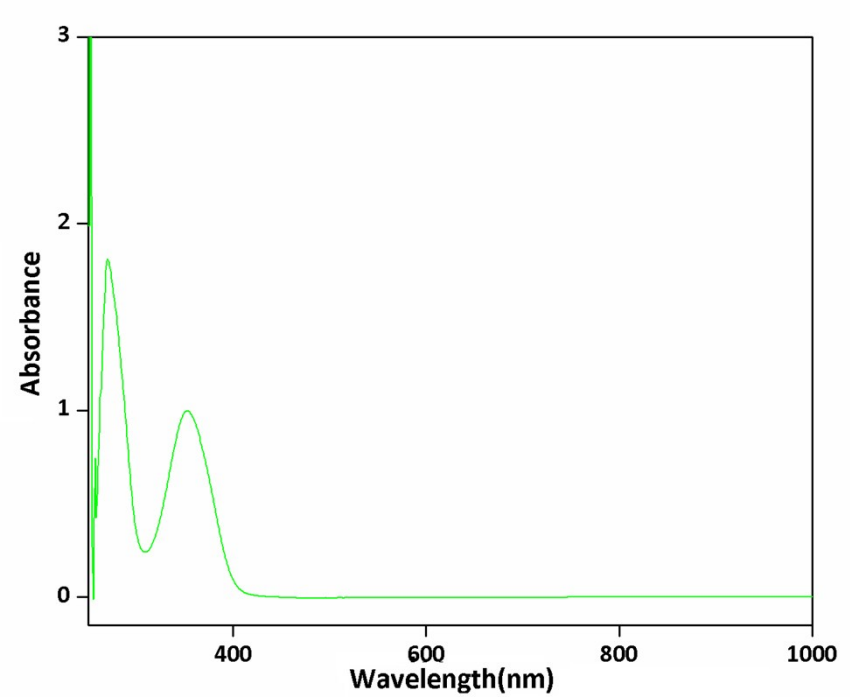

Fig. S5: UV-Vis spectrum of complex **1** in DMF.

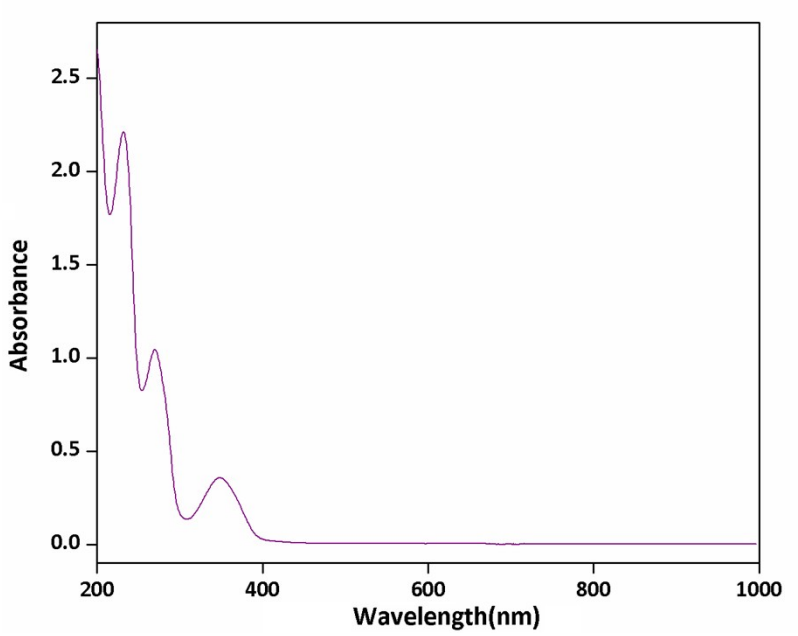

Fig. S6: UV-Vis spectrum of complex **2** in acetonitrile.

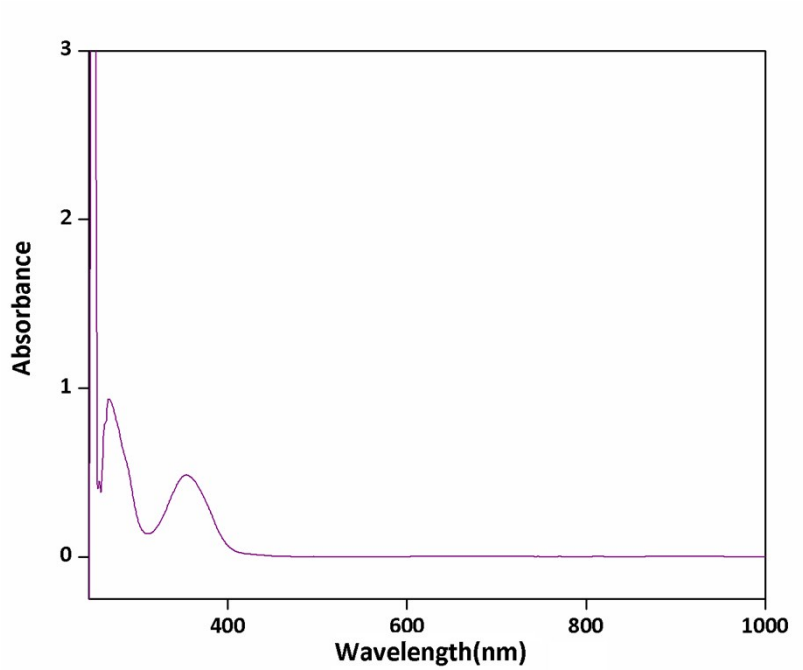

Fig. S7: UV-Vis spectrum of complex **3** in DMF.

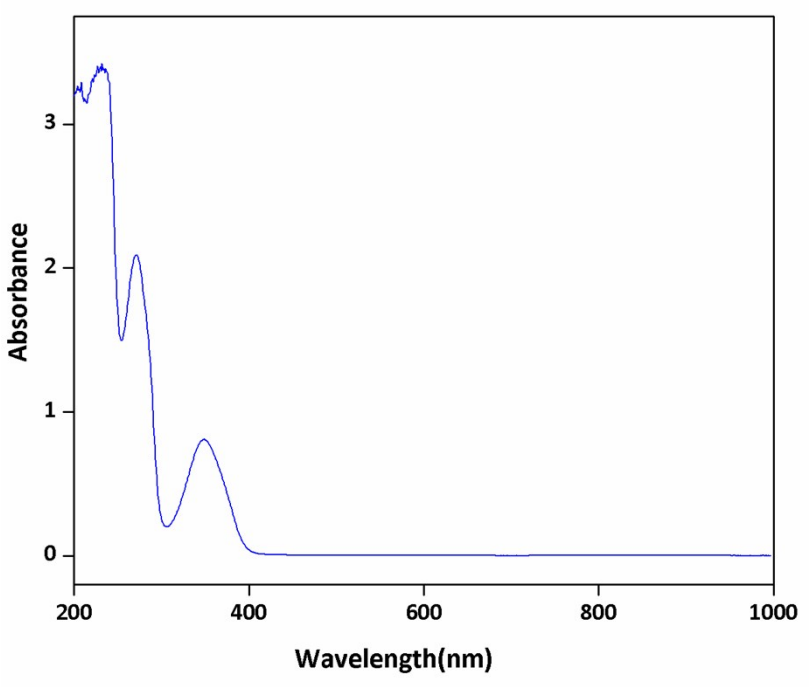

Fig. S8: UV-Vis spectrum of complex **4** in acetonitrile.

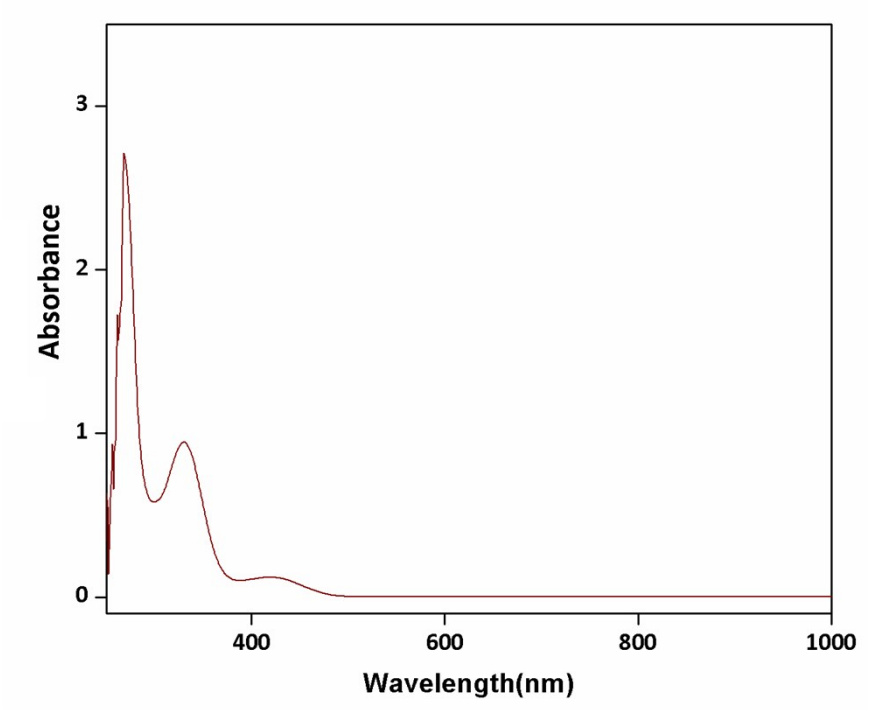

Fig. S9: UV-Vis spectrum of H_2L^1 in DMF.

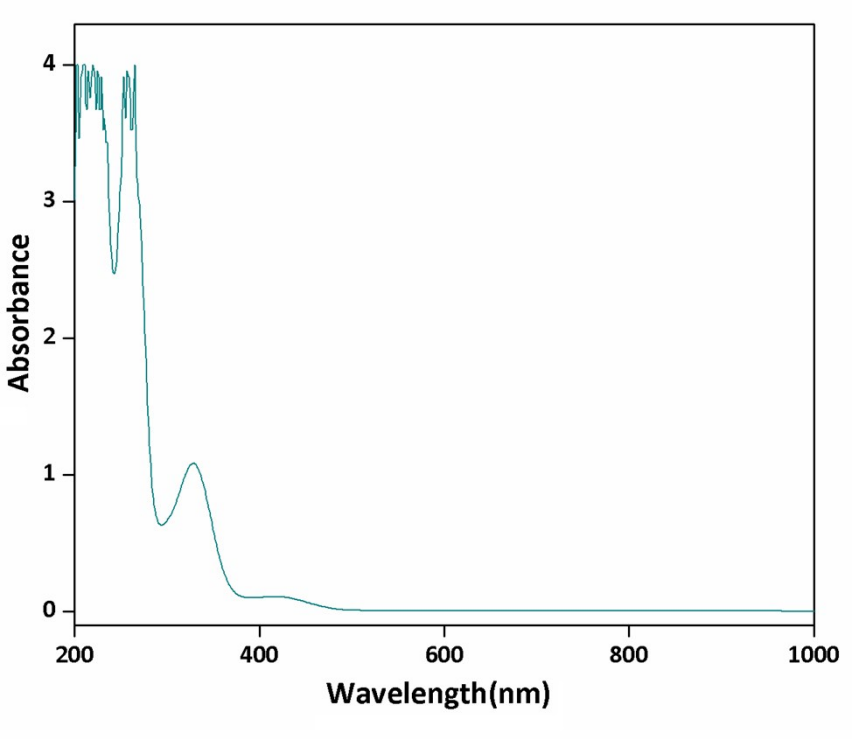

Fig. S10: UV-Vis spectrum of H_2L^2 in acetonitrile.

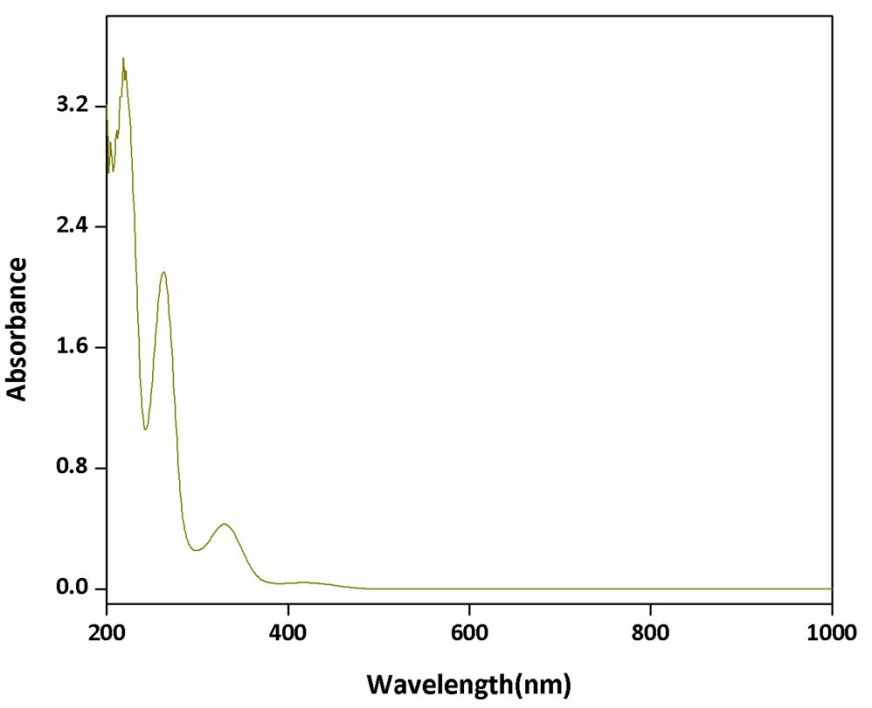

Fig. S11: UV-Vis spectrum of H_2L^3 in acetonitrile.

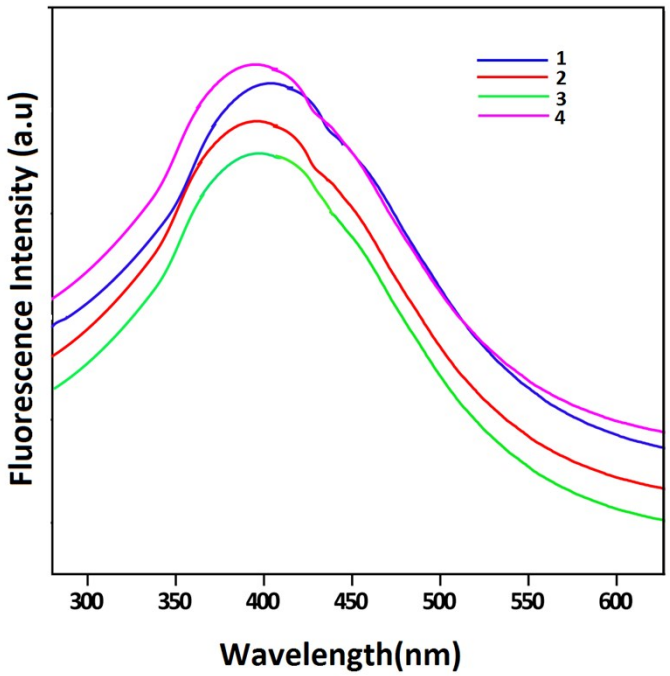

Fig. S12: Fluorescence spectra of complexes **1**-**4**.

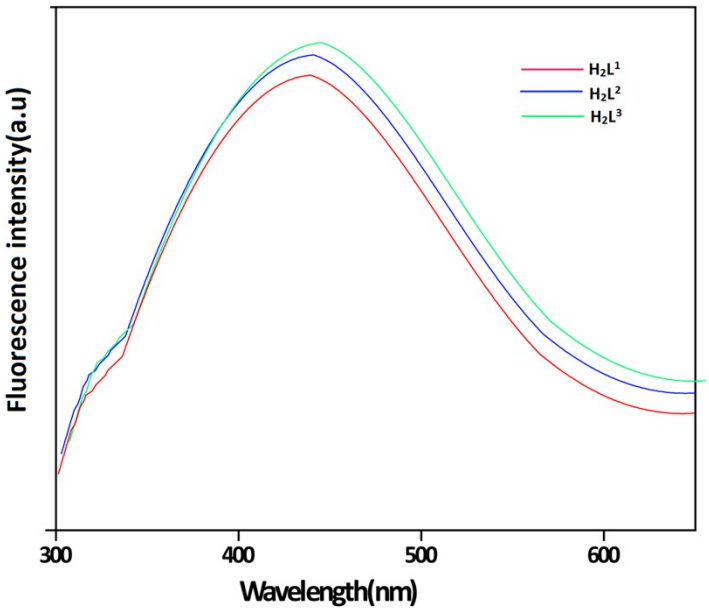

Fig. S13: Fluorescence spectra of ligands.

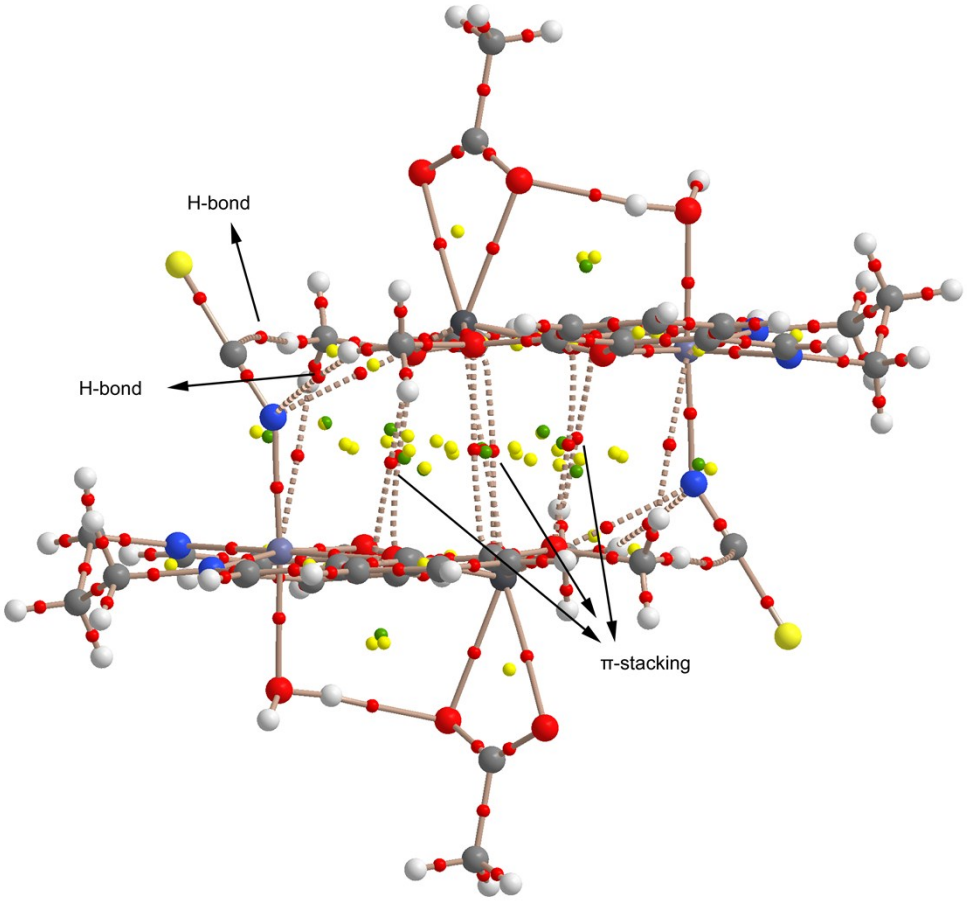

Fig. S14: Complete AIM analyses of the dimers of complex **1**.