Electronic supplementary information (ESI)

Metal-organic Architectures Driven by a Multifunctional 6-Aminouracil Spacer: Structures, Noncovalent Interactions, and Conductivity

Atanu Purkayastha,[a] Sourab Dhar,[b] Suvra Prakash Mondal,[b] Antonio Franconetti,[c] Antonio Frontera,*[c] Rakesh Ganguly,*[d] Alexander M. Kirillov,*[e,f] Tarun Kumar Misra*[a]

[a.] *Department of Chemistry, National Institute of Technology Agartala, Tripura 799046, India; E-mail: tkmisra.chem@nita.ac.in / tkmisra70@yahoo.com*
[b.] *Department of Physics, National Institute of Technology Agartala, Tripura 799046, India*
[c.] *Departamento de Química, Universitat de les llles Balears, Crta. de Valldemossa 07122, Spain; E-mail: toni.frontera@uib.es*
[d.] *Division of Chemistry & Biological Chemistry, Nanyang Technology University, Singapore 639798; E-mail: rganguly@ntu.edu.sg*
[e.] *Centro de Química Estrutural, Instituto Superior Técnico, Universidade de Lisboa, Av. Rovisco Pais, 1049-1005, Lisbon, Portugal; E-mail: kirillov@tecnico.ulisboa.pt*
[f.] *Research Institute of Chemistry, Peoples' Friendship University of Russia (RUDN University), 6 Miklukho-Maklaya st., Moscow, 117198, Russian Federation*

Supplementary Figures

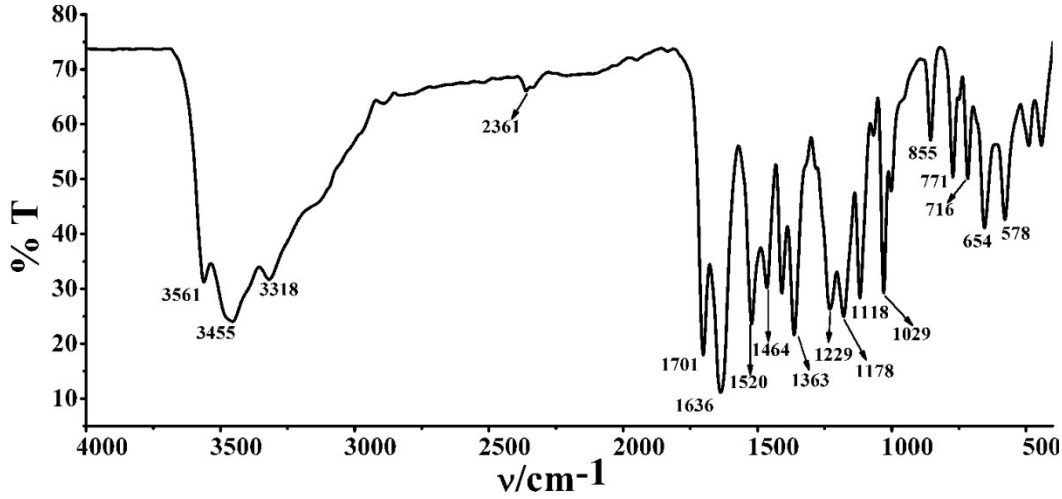

Figure S1: IR spectrum of **1**.

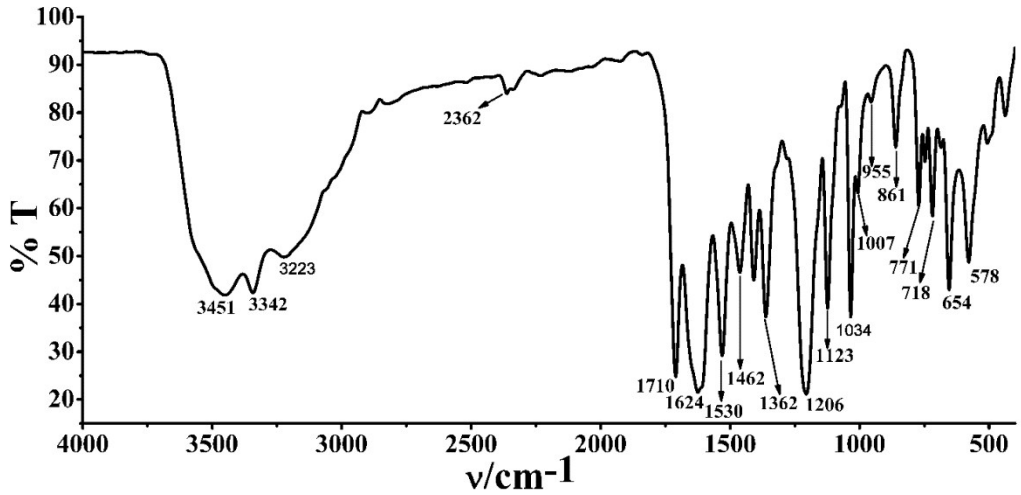

Figure S2: IR spectrum of **2**.

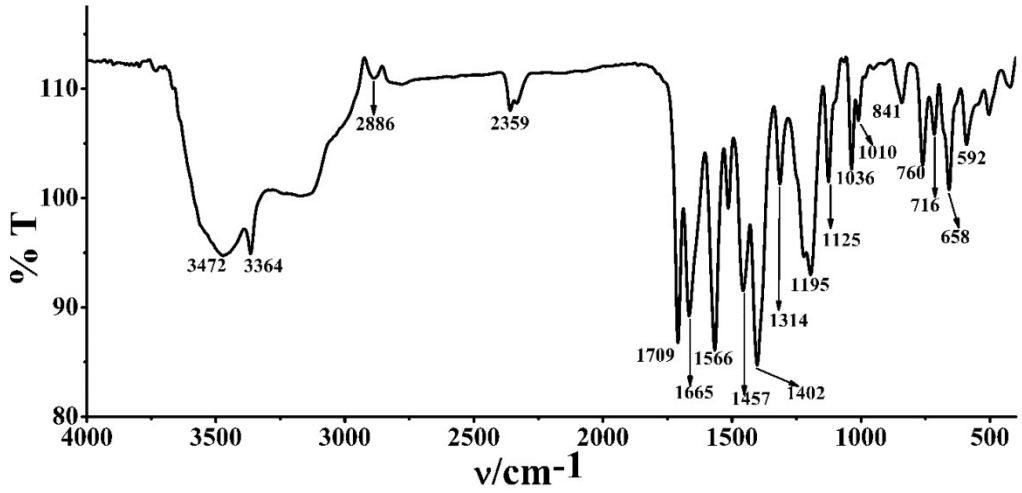

Figure S3: IR spectrum of **3**.

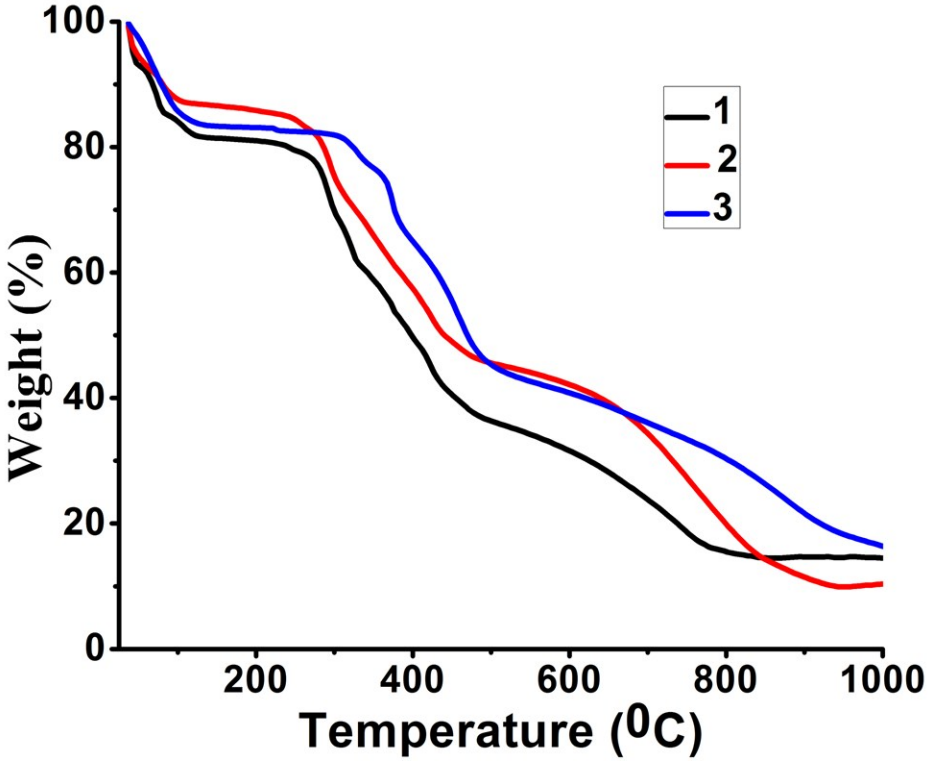

Figure S4: TGA plots of **1-3**.

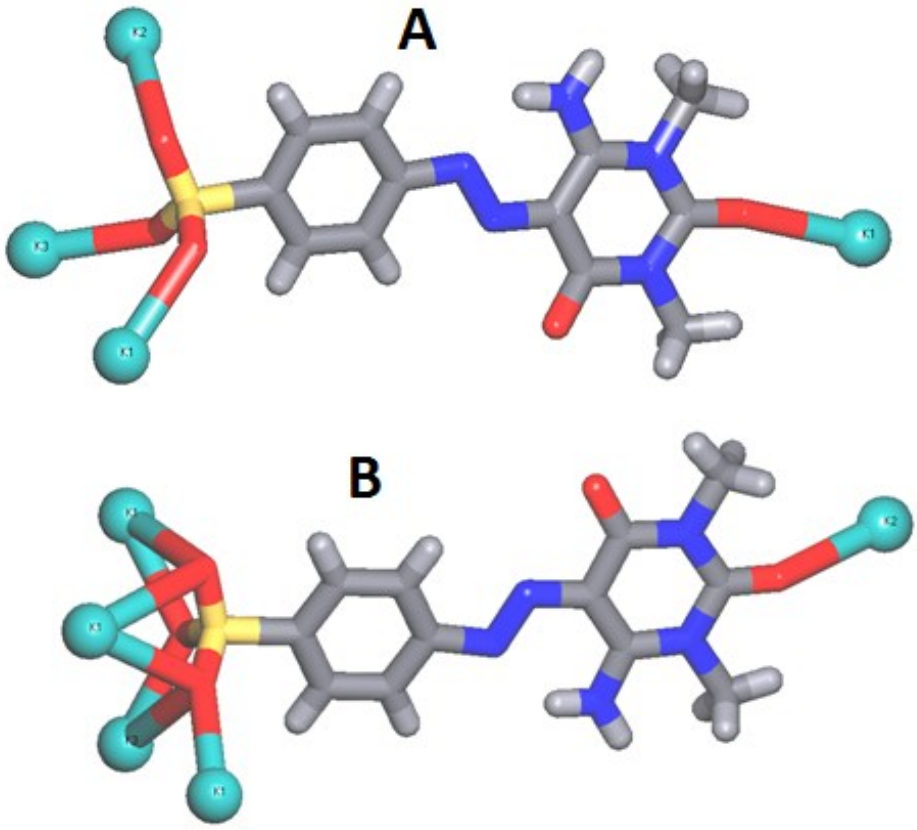

Figure S5: Connectivity of (**A**) μ_4-H_2L^-(top) and (**B**) μ_5-H_2L^- (bottom) blocks in compound **2**.

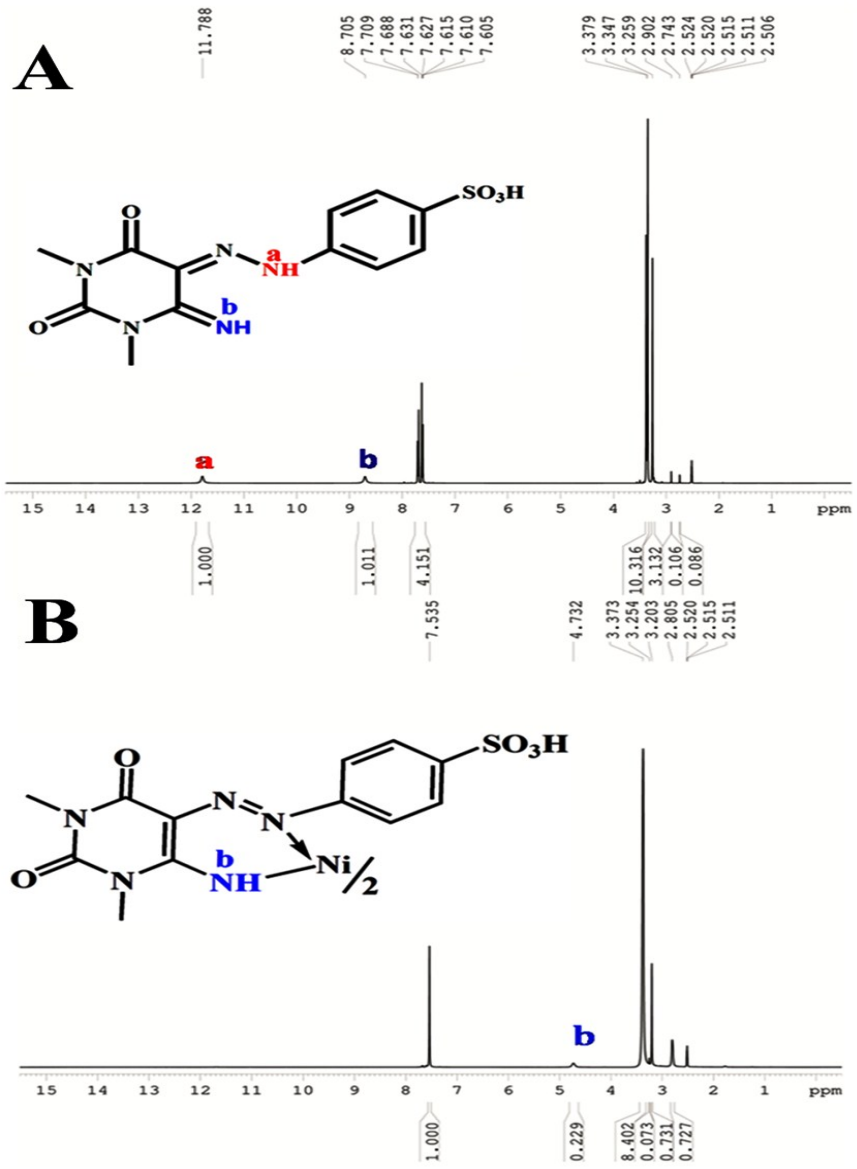

Figure S6: ^{1}H NMR spectra of **1** (**A**) and **3** (**B**).

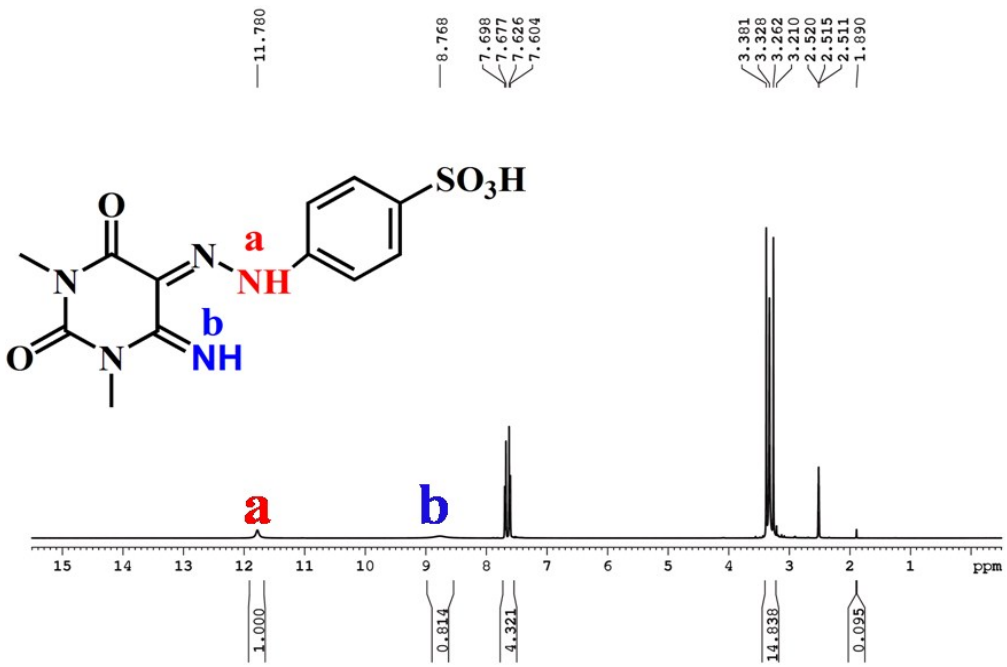

Figure S7: [1]H NMR spectrum of **2**.

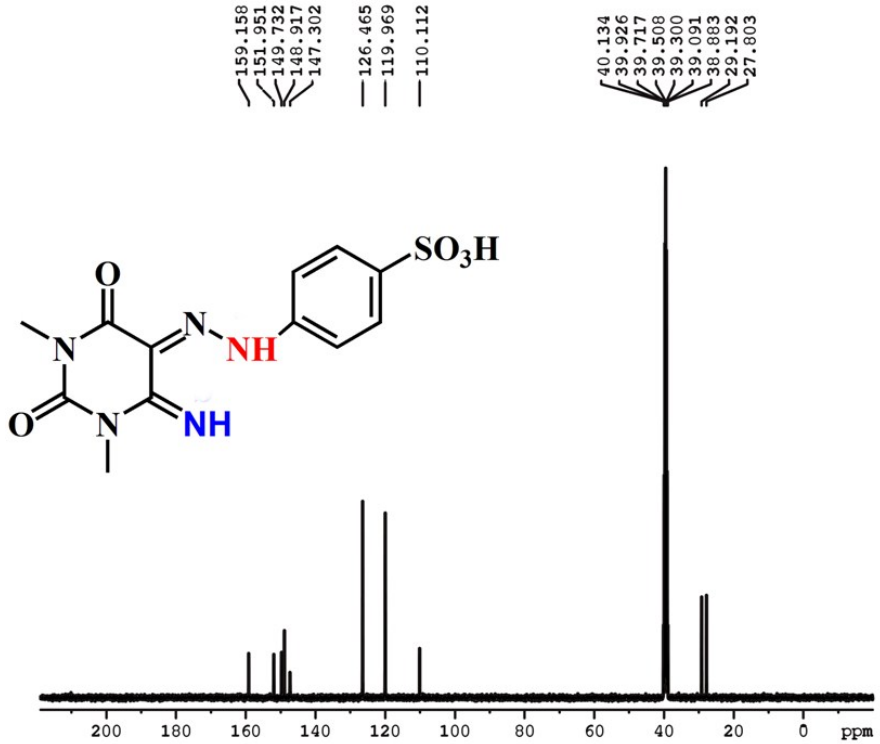

Figure S8: [13]C NMR spectrum of **1**.

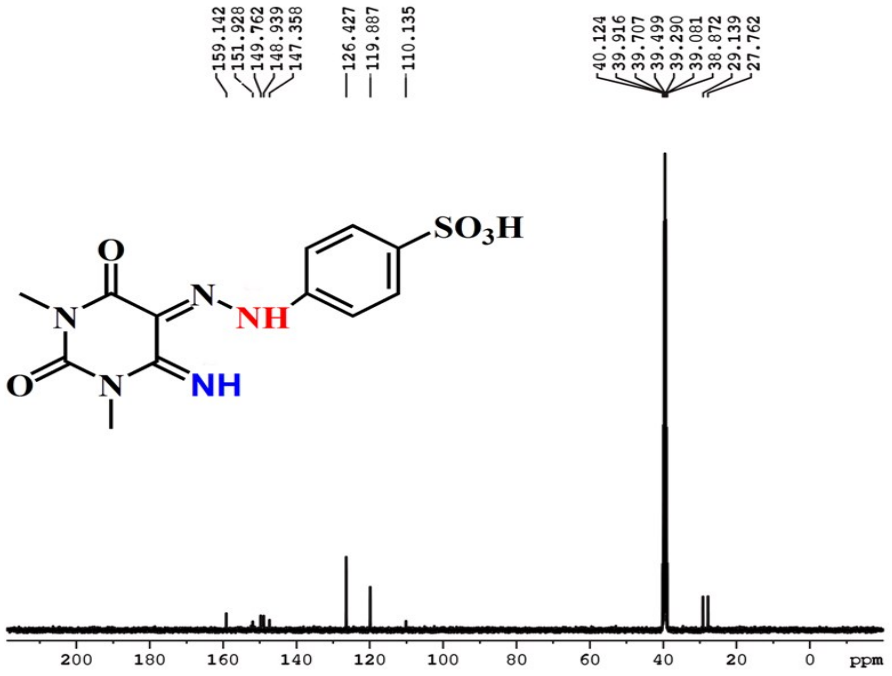

Figure S9: ^{13}C NMR spectrum of **2**.

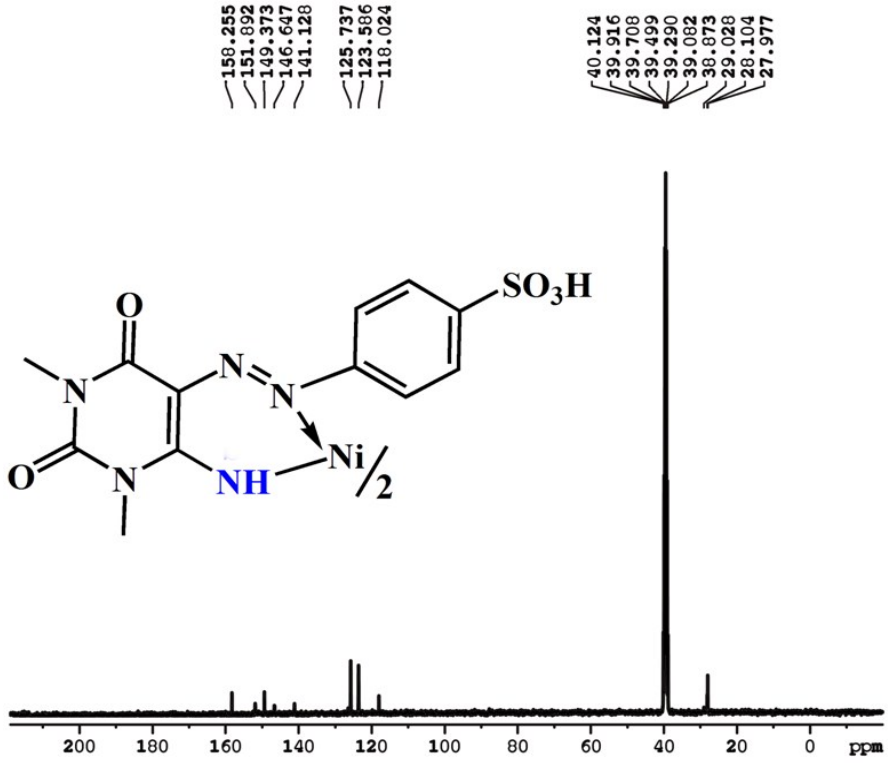

Figure S10: ^{13}C NMR spectrum of **3**.

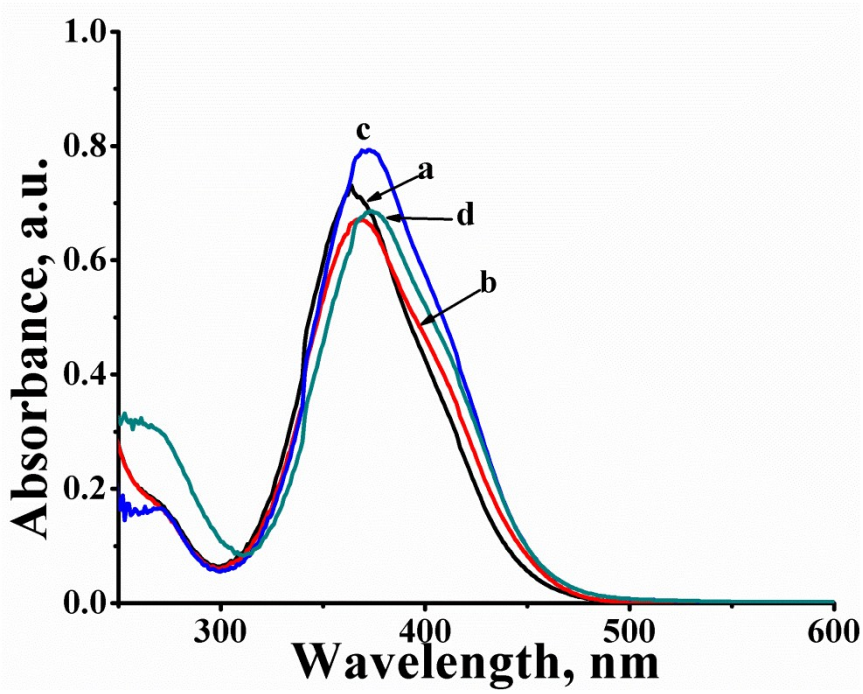

Figure S11: UV-vis spectra of **1** in (a) MeOH, (b) EtOH, (c) DMF and (d) DMSO.

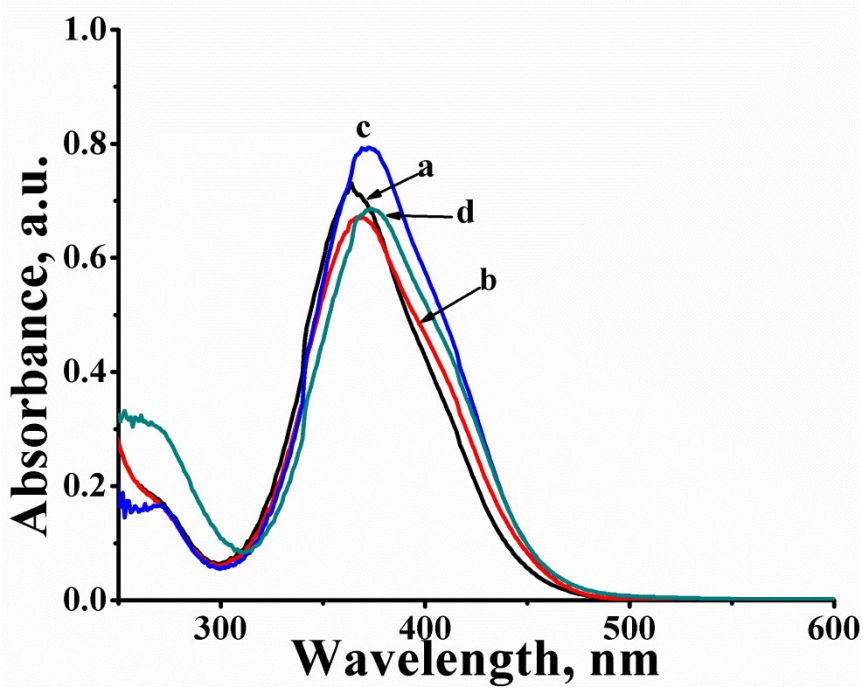

Figure S12: UV-vis spectra of **2** in (a) MeOH, (b) EtOH, (c) DMF and (d) DMSO.

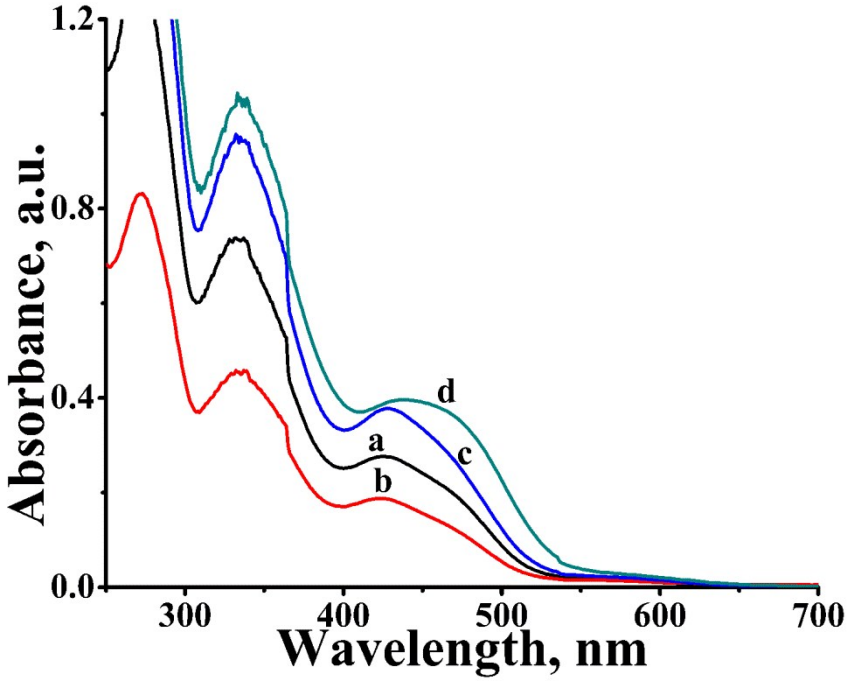

Figure S13: UV-vis spectra of **3** in (a) MeOH, (b) EtOH, (c) DMF and (d) DMSO.

Supplementary Tables

Table S1. Bond lengths (Å) for **1**.

O3-S1	1.430(4)	O3-Na1^{i}	2.361(4)
O4-S1	1.453(4)	O5-S1	1.454(4)
S1-C11	1.763(4)	Na1-O6	2.303(4)
Na1-O2	2.353(3)	Na1-O3^{ii}	2.360(4)
Na1-O7	2.361(4)	Na1-O8	2.385(3)
Na1-N2	3.020(4)	C1-N2	1.382(5)
C1-C2	1.417(6)	C1-C7	1.427(6)
C2-N3	1.317(6)	C2-N4	1.373(5)
C3-N4	1.473(6)	C4-O1	1.211(5)
C4-N5	1.379(6)	C4-N4	1.389(6)
N5-C7	1.388(5)	N5-C6	1.468(6)
C7-O2	1.240(5)	C8-C9	1.389(6)
C8-C13	1.399(6)	C8-N1	1.432(5)
C9-C10	1.390(6)	C10-C11	1.388(6)
C11-C12	1.400(6)	C12-C13	1.380(6)
N1-N2	1.277(5)		

^{i}2-X, ½+Y, ½-Z, ^{ii}2-X, -½+Y, ½-Z

Table S2. Bond angles (°) for **1**.

S1-O3-Na1^{i}	128.4(2)	O3-S1-O4	112.5(3)

O3-S1-O5	114.2(3)	O4-S1-O5	110.8(3)
O3-S1-C11	106.8(2)	O4-S1-C11	105.9(2)
O5-S1-C11	106.1(2)	O6-Na1-O2	91.08(14)
O6-Na1-O3^{ii}	79.36(14)	O2-Na1-O3^{ii}	169.03(16)
O6-Na1-O7	170.79(14)	O2-Na1-O7	90.01(13)
O^{ii}-Na1-O7	100.29(15)	O6-Na1-O8	104.30(14)
O2-Na1-O8	80.90(12)	O3^{ii}-Na1-O8	96.16(15)
O7-Na1-O8	84.91(12)	O6-Na1-N2	95.55(13)
O2-Na1-N2	58.54(11)	O3^{ii}-Na1-N2	127.25(15)
O7-Na1-N2	77.25(11)	O8-Na1-N2	135.09(12)
N2-C1-C2	126.6(4)	N2-C1-C7	113.2(4)
C2-C1-C7	120.1(4)	N3-C2-N4	118.7(4)
N3-C2-C1	122.4(4)	N4-C2-C1	118.9(4)
O1-C4-N5	122.2(4)	O1-C4-N4	120.9(4)
N5-C4-N4	116.9(4)	C4-N5-C7	124.4(4)
C4-N5-C6	118.2(4)	C7-N5-C6	117.3(4)
O2-C7-N5	118.8(4)	O2-C7-C1	124.7(4)
N5-C7-C1	116.5(4)	C9-C8-C13	120.5(4)
C9-C8-N1	124.5(4)	C13-C8-N1	115.0(4)
C8-C9-C10	119.8(4)	C11-C10-C9	119.7(4)
C10-C11-C12	120.5(4)	C10-C11-S1	120.1(3)
C12-C11-S1	119.4(3)	C13-C12-C11	119.8(4)
C12-C13-C8	119.6(4)	N2-N1-C8	112.5(3)
N1-N2-C1	117.5(3)	N1-N2-Na1	134.0(3)
C1-N2-Na1	101.3(2)	C2-N4-C4	122.8(4)
C2-N4-C3	120.0(4)	C4-N4-C3	117.2(4)
C7-O2-Na1	121.4(3)		

^{i}2-X, ½+Y, ½-Z, ^{ii}2-X, -½+Y, ½-Z

Table S3. Bond lengths (Å) for **2**.

C1-C6	1.386(3)	C1-C2	1.394(3)
C1-S1	1.772(2)	C2-C3	1.383(3)
C3-C4	1.397(3)	C4-C5	1.394(3)
C4-N1	1.421(3)	C5-C6	1.398(3)
C7-N2	1.373(3)	C7-C10	1.413(3)

C7-C8	1.435(3)	C8-O7	1.237(3)
C8-N3	1.395(3)	C9-O8	1.214(2)
C9-N3	1.382(3)	C9-N4	1.394(3)
C10-N5	1.315(3)	C10-N4	1.371(3)
C11-N3	1.471(3)	C12-N4	1.469(3)
C13-C14	1.385(3)	C13-C18	1.397(3)
C13-S2	1.778(2)	C14-C15	1.391(3)
C15-C14	1.391(3)	C15-C16	1.391(3)
C16-C17	1.396(3)	C16-N6	1.428(3)
C17-C18	1.392(3)	C18-C13	1.398(4)
C19-N7	1.373(3)	C19-C22	1.414(3)
C19-C20	1.442(3)	C20-O9	1.239(2)
C20-N8	1.390(3)	C21-O10	1.214(2)
C21-N8	1.380(3)	C21-N9	1.392(3)
C22-N10	1.322(3)	C22-N9	1.369(3)
C23-N8	1.469(3)	C24-N9	1.470(3)
K1-O6	2.6836(18)	K1-O8^{iii}	2.6863(15)
K1-O1	2.7305(19)	K1-O4	2.8491(19)
K1-O6^{iv}	2.9660(19)	K1-O11	3.098(5)
K1-O5	3.183(3)	K1-O5^{iv}	3.190(2)
K1-S2^{iv}	3.5127(17)	K1-S2	3.5719
K1-K1	4.3455(11)	K1-K3	4.6278(12)
K2-O12A	2.629(11)	K2-O12A^{v}	2.629(11)
K2-O10	2.7412(15)	K2-O10^{v}	2.7412(15)
K2-O2^{v}	2.7517(18)	K2-O2	2.7517(18)
K2-O12^{v}	2.806(2)	K2-O12	2.806(2)
N1-N2	1.281(2)	N6-N7	1.283(2)
O1-S1	1.4524(18)	O2-S1	1.4488(17)
O3-S1	1.4443(18)	O4-S2	1.453(2)
O4-K3	2.522(3)	O5-S2	1.451(2)
O5-K1	3.191(2)	O6-S2	1.4540(18)
O6-K1	2.684(2)	O6-K1	2.966(2)
O8-C9	1.213(3)	O13-K3	2.592(5)
K3-S2	3.5237(13)	K1-S2	3.5719(9)

^{i}-x+1/2, y-1/2, z+3/2; ^{ii}x, -y+1/2, z-1/2; ^{iii}-x+1/2, y+1/2, -z+3/2; ^{iv}-x, y,-z+3/2; ^{v}-x, y, -z+1/2; ^{vi}-x, -y+1, -z+1;^{vii}x, -y+1, z+1/2

Table S4. Bond angles (°) for **2**.

C6-C1-C2	120.69(19)	C6-C1-S1	122.46(16)

C2-C1-S1	116.83(16)	C3-C2-C1	120.5(2)
C2-C3-C4	119.26(19)	C5-C4-C3	120.18(19)
C5-C4-N1	116.27(19)	C3-C4-N1	123.53(19)
C4-C5-C6	120.39(19)	C1-C6-C5	118.94(19)
N2-C7-C10	125.49(18)	N2-C7-C8	114.35(18)
C10-C7-C8	120.16(18)	O7-C8-N3	119.10(19)
O7-C8-C7	124.69(19)	N3-C8-C7	116.19(18)
O8-C9-N3	122.62(19)	O8-C9-N4	121.02(19)
N3-C9-N4	116.36(17)	N5-C10-N4	118.73(18)
N5-C10-C7	122.22(19)	N4-C10-C7	119.05(18)
C14-C13-C18	120.3(2)	C14-C13-S2^{i}	121.0(2)
C18-C13-S2^{i}	118.7(2)	C13-C14-C15	120.4(2)
C14-C15-C16	119.7(2)	C15-C16-C17	119.79(19)
C15-C16-N6	124.64(19)	C17-C16-N6	115.57(18)
C18-C17-C16	120.5(2)	C17-C18-C13	119.2(2)
N7-C19-C22	126.69(18)	N7-C19-C20	113.89(17)
C22-C19-C20	119.42(18)	O9-C20-N8	119.30(19)
O9-C20-C19	124.04(19)	N8-C20-C19	116.66(18)
O10-C21-N8	121.8(2)	O10-C21-N9	121.6(2)
N8-C21-N9	116.61(19)	N10-C22-N9	119.0(2)
O6-K1-O8	77.94(5)	N9-C22-C19	118.97(19)
O8^{iii}-K1-O1	84.66(5)	O6^{ii}-K1-O1	105.34(7)
O6^{ii}-K1-O4	98.41(7)		
O8-K1-O4	68.63(5)	O4-K1-O6^{iv}	71.78(7)
O6^{ii}-K1-O6^{iv}	79.55(6)	O8^{iii}-K1-O11	102.44(9)
O1-K1-O6^{iv}	144.18(7)	O4-K1-O11	97.20(10)
O6^{ii}-K1-O11	163.30(10)	O6^{ii}-K1-O5	140.11(6)
O1-K1-O11	58.38(9)	O1-K1-O5	96.94(6)
O6^{iv}-K1-O11	111.12(9)	O6-K1-O5	101.12(6)
O8-K1-O5	71.59(5)	O8^{iii}-K1-O5^{iv}	149.92(7)
O4-K1-O5	46.70(6)	O4-K1-O5^{iv}	85.00(7)
O6^{ii}-K1-O5^{iv}	121.63(5)	O5-K1-O5^{iv}	79.90(6)
O1-K1-O5^{iv}	108.58(7)	O8^{iii}-K1-S2^{iv}	138.37(4)
O6^{iv}-K1-O5^{iv}	46.11(5)	O4-K1-S2^{iv}	22.80(5)
O6^{ii}-K1-S2^{iv}	103.58(4)	O11-K1-S2	75.58(8)
O1-K1-S2^{iv}	132.39(5)	O5-K1-S2	23.93(4)
O6-K1-S2	86.59(5)	O8^{iii}-K1-S2	67.33(4)
O5-K1-S2	82.73(6)	O4-K1-S2	22.80(5)
O6^{ii}-K1-S2	118.94(5)	O11-K1-S2	75.58(8)
O1-K1-S2	118.84(4)	O5^{iv}-K1-S2	82.73(6)

O6^{iv}-K1-S2	86.59(5)	O12A^{v}-K2-O10	88.0(3)
O5^{iv}-K1-S2^{iv}	24.40(4)	O12A-K2-O10	101.4(3)
S2^{iv}-K1-S2	76.5	O10-K2-O10^{v}	169.56(8)
O12A-K2-O10	101.4(3)	O12A-K2-O2	148.6(4)
O12A-K2-O10	88.0(3)	O10^{v}-K2-O2^{v}	89.62(5)
O12A-K2-O2	97.0(4)	O12A-K2-O2	97.0(4)
O10-K2-O2^{v}	84.69(5)	O10^{v}-K2-O2	84.69(5)
O12A^{v}-K2-O2	148.6(4)	O10-K2-O12^{v}	94.88(4)
O10-K2-O2	89.62(5)	O2^{v}-K2-O12^{v}	79.14(6)
O2^{v}-K2-O2	114.01(8)	O10-K2-O12	92.63(4)
O10^{v}-K2-O12^{v}	92.63(4)	N1-N2-C7	118.09(17)
O2^{v}-K2-O12	166.50(7)	C9-N3-C11	117.43(17)
O10^{v}-K2-O12	94.88(5)	C10-N4-C9	123.27(17)
N2-N1-C4	113.49(17)	C9-N4-C12	117.27(17)
C9-N3-C8	124.87(18)	N7-N6-C16	112.89(17)
C8-N3-C11	117.69(17)	C21-N8-C20	124.64(18)
C10-N4-C12	119.34(17)	C20-N8-C23	119.22(18)
O1-K1-O4	139.47(6)	C22-N9-C24	119.53(18)
O8^{iii}-K1-O6^{iv}	130.41(6)	S1-O1-K1	130.97(11)
S2-O4-K3	122.56(11)	S2-O5-K1	93.25(14)
K3-O4-K1	118.87(7)	K1-O5-K1	99.97(7)
S2-O5-K1^{iv}	90.33(10)	S2-O6-K1^{iv}	99.53(9)
S2-O6-K1^{vii}	159.59(11)	C9-O8-K1	167.92(15)
K1^{vii}-O6-K1^{iv}	100.45(6)	O13-K3-S2	109.16(9)
C21-O10-K2	156.71(15)	O3-S1-O2	113.65(11)
O4-K3-S2	22.05(5)	O2-S1-O1	112.80(12)
O3-S1-O1	112.48(12)	O2-S1-C1	106.91(10)
O3-S1-C1	105.36(10)	O5-S2-O4	112.13(14)
O1-S1-C1	104.75(10)	O4-S2-O6	112.25(13)
O5-S2-O6	112.78(14)	O4-S2-C13^{iii}	105.72(12)
O5-S2-C13^{iii}	106.40(12)	O5-S2-K1^{iv}	65.27(8)
O6-S2-C13^{iii}	106.98(10)	O6-S2-K1^{iv}	56.38(8)
O4-S2-K1^{iv}	104.75(8)	O4-S2-K3	37.10(8)
C13^{iii}-S2-K1^{iv}	149.22(9)	C13^{iii}-S2-K3	111.30(9)
O6-S2-K3	75.83(10)	O5-S2-K1	62.82(1)
K1^{iv}-S2-K3	90.69(2)	O6-S2-K1	135.88(8)
O4-S2-K1	49.42(9)	K1^{iv}-S2-K1	87.087(17)
C13^{iii}-S2-K1	116.43(7)		
K3-S2-K1	81.41(3)		
N6-N7-C19	118.37(17)		

C21-N8-C23	116.14(17)		
C22-N9-C21	123.15(18)		
C21-N9-C24	117.31(17)		
S1-O2-K2	128.50(11)		
S2-O4-K1	107.78(12)		

[i]-x+1/2, y-1/2, z+3/2 [ii]x, -y+1/2, z-1/2 [iii]-x+1/2, y+1/2, -z+3/2; [iv]-x, y,-z+3/2 [v]-x, y, -z+1/2[vi]-x, -y+1, -z+1; [vii]x, -y+1, z+1/2

Table S5. Bond lengths (Å) for **3**.

Ni1-N3[i]	1.8548(12)	Ni1-N3	1.8548(12)
Ni1-N1[i]	1.8937(13)	Ni1-N1	1.8937(13)
Na1-O9A	2.335(8)	Na1-O8A	2.338(7)
Na1-O9B	2.343(5)	Na1-O8B	2.372(5)
Na1-O7	2.3933(13)	Na1-O10	2.4112(14)
Na1-O11	2.4624(14)	Na1-O11[ii]	2.4339(14)
Na1-Na1	3.5970(13)	C1-C2	1.422(3)
C1-N2	1.3412(18)	C2-N3	1.299(2)
C1-C6	1.449(2)	C3-N4	1.468(2)
C2-N4	1.3871(18)	C4-N4	1.3834(19)
C4-O7	1.2181(18)	C5-N5	1.4726(19)
C4-N5	1.386(2)	C6-N5	1.3836(19)
C6-O6	1.232(2)	C7-C8	1.396(2)
C7-C12	1.389(2)	C8-C9	1.389(2)
C7-N1	1.4493(18)	C10-C11	1.390(2)
C9-C10	1.391(2)	C11-C12	1.387(2)
C10-S1	1.7751(15)	O3-S1	1.4526(12)
N1-N2	1.2944(17)	O5-S1	1.455(12)
O4-S1	1.4577(13)		

[i]1-X, 1-Y, 2-Z, [ii]1-X, -Y, 1-Z

Table S6. Bond angles (°) for **3**.

N3[i]-Ni1-N3	180.00	N3[i]-Ni1-N1	90.84(6)

N3[i]-Ni1-N1[i]	89.16(6)	N3-Ni1-N1	90.84(6)
N3-Ni1-N1[i]	89.16(6)	N1[i]-Ni1-N1	180.0
O9A-Na1-O8A	163.1(3)	O9A-Na1-O7	88.5(3)
O9B-Na1-O8B	168.2(2)	O9B-Na1-O7	83.81(17)
O8A-Na1-O7	88.8(4)	O9A-Na1-O10	104.0(3)
O8B-Na1-O7	99.24(16)	O9B-Na1-O10	92.8(3)
O7-Na1-O10	84.07(5)	O8A-Na1-O10	92.3(3)
O8B-Na1-O10	98.89(16)	O8A-Na1-O11	106.4(4)
O9A-Na1-O11	80.28(8)	O8B-Na1-O11	99.48(9)
O9B-Na1-O11	78.4(3)	O10-Na1-O11	90.25(5)
O7-Na1-O11	164.02(5)	O8A-Na1-O11[ii]	86.4(3)
O9A-Na1-O11[ii]	84.19(10)	O8B-Na1-O11[ii]	86.4(3)
O9B-Na1-O11[ii]	78.4(3)	O10-Na1-O11[ii]	174.90(7)
O7-Na1-O11[ii]	100.80(5)	O11-Na1-O11[ii]	85.44(7)
O8A-Na1-Na1[ii]	98.5(4)	O9A-Na1-Na1[ii]	79.43(9)
O10-Na1-Na1[ii]	133.22(4)	O7-Na1-Na1[ii]	141.15(5)
O11[ii]-Na1-Na1[ii]	42.41(3)	O11-Na1-Na1[ii]	43.03(3)
N2-C1-C2	124.47(13)	N2-C1-C6	114.04(14)
C2-C1-C6	120.78(13)	C11-C10-S1	119.53(12)
C11-C10-C9	120.61(14)	C12-C11-C10	119.99(15)
C9-C10-S1	119.86(11)	N2-N1-C7	109.47(12)
C11-C12-C7	119.49(14)	C7-N1-Ni1	122.04(9)
N2-N1-Ni1	128.70(10)	C2-N3-Ni1	128.87(12)
N1-N2-C1	122.03(13)	C4-N4-C3	116.94(12)
C4-N4-C2	122.70(14)	C6-N5-C4	124.72(18)
C2-N4-C3	120.32(13)	C4-N5-C5	116.30(13)
C6-N5-C5	118.74(14)	Na1-O11-Na1[ii]	94.55(5)
C4-O7-Na1	152.35(11)	O3-S1-O4	111.44(8)
O3-S1-O5	112.80(7)	O3-S1-C10	106.93(7)
O5-S1-O4	113.04(7)	O4-S1-C10	105.73(7)
O5-S1-C10	106.30(7)		

[i]1-X, 1-Y, 2-Z, [ii]1-X, -Y, 1-Z