Electronic Supplementary Material (ESI) for CrystEngComm

{[$Co_2(ndc)_2(bpee)_2$](bpee)}: A 3D Multifunctional MOF

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Table S1: Bond Distances of **Complex1**

Bonds	Bond distances	Bonds	Bond distances
Co1 -O1	2.232(4)	N5 -C54	1.3897
Co1 -O2	2.151(3)	N5 -C52	1.3893
Co1 -O5	2.056(3)	N6 -C59	1.267(15)
Co1 -N1	2.160(4)	N6 -C61	1.258(16)
Co1 -O7_a	2.015(3)	C1 -C2	1.368(8)
Co1 -N2_e	2.147(3)	C2 -C3	1.395(7)
Co2 -O6	2.012(3)	C3 -C6	1.475(7)
Co2 -N3	2.144(4)	C3 -C4	1.379(7)
Co2 -O8_a	2.044(3)	C4 -C5	1.364(8)
Co2 -O3_d	2.213(4)	C6 -C7	1.322(7)
Co2 -O4_d	2.147(3)	C7 -C8	1.468(7)
Co2 -N4_e	2.140(4)	C8 -C9	1.406(7)
O1 -C13	1.257(6)	C8 -C12	1.389(7)
O2 -C13	1.268(6)	C9 -C10	1.337(7)
O3 -C24	1.234(6)	C11 -C12	1.351(6)
O4 -C24	1.274(6)	C13 -C14	1.487(7)
O5 -C25	1.276(5)	C14 -C19	1.340(7)
O6 -C25	1.246(5)	C14 -C15	1.408(7)
O7 -C36	1.247(6)	C15 -C16	1.357(7)
O8 -C36	1.253(6)	C16 -C17	1.400(7)
N1 -C1	1.327(7)	C17 -C20	1.424(7)
N1 -C5	1.327(6)	C17 -C18	1.412(7)
N2 -C10	1.343(6)	C18 -C19	1.420(7)
N2 -C11	1.338(6)	C18 -C23	1.410(7)
N3 -C37	1.339(7)	C20 -C21	1.359(7)
N3 -C41	1.326(7)	C21 -C24	1.510(7)
N4 -C46	1.331(6)	C21 -C22	1.410(7)
N4 -C47	1.345(6)	C22 -C23	1.371(7)
C25 -C26	1.494(7)	C6 -H6	0.9300
C26 -C31	1.433(7)	C7 -H7	0.9300
C26 -C27	1.365(6)	C9 -H9	0.9300
C27 -C28	1.419(6)	C10 -H10	0.9300
C28 -C35	1.411(7)	C11 -H11	0.9300
C28 -C29	1.413(7)	C12 -H12	0.9300
C29 -C30	1.434(7)	C15 -H15	0.9300

C29 -C32	1.420(7)	C16 -H16	0.9300
C30 -C31	1.364(7)	C19 -H19	0.9300
C32 -C33	1.367(6)	C20 -H20	0.9300
C33 -C36	1.505(7)	C22 -H22	0.9300
C33 -C34	1.409(7)	C23 -H23	0.9300
C34 -C35	1.360(7)	C27 -H27	0.9300
C37 -C38	1.378(8)	C30 -H30	0.9300
C38 -C39	1.372(8)	C31 -H31	0.9300
C39 -C40	1.394(9)	C32 -H32	0.9300
C39 -C42	1.483(8)	C34 -H34	0.9300
C40 -C41	1.396(8)	C35 -H35	0.9300
C42 -C43	1.263(9)	C37 -H37	0.9300
C43 -C44	1.470(8)	C38 -H38	0.9300
C44 -C48	1.362(7)	C40 -H40	0.9300
C44 -C45	1.403(7)	C41 -H41	0.9300
C45 -C46	1.383(8)	C42 -H42	0.9300
C47 -C48	1.395(8)	C43 -H43	0.9300
C1 -H1	0.9300	C45 -H45	0.9300
C2 -H2	0.9300	C46 -H46	0.9300
C4 -H4	0.9300	C47 -H47	0.9300
C5 -H5	0.9300	C48 -H48	0.9300
C49 -C50	1.62(2)	C56 -C57	1.631(16)
C49 -C49_g	1.21(2)	C56 -C56_h	1.130(17)
C50 -C55	1.3897	C57 -C58	1.387(14)
C50 -C51	1.3909	C57 -C62	1.399(15)
C51 -C52	1.3906	C58 -C59	1.330(16)
C54 -C55	1.3895	C61 -C62	1.375(18)
C49 -H49	0.9300	C56 -H56	0.9300
C51 -H51	0.9300	C58 -H58	0.9300
C52 -H52	0.9300	C59 -H59	0.9300
C54 -H54	0.9300	C61 -H61	0.9300
C55 -H55	0.9300	C62 -H62	0.9300

***a = -1+x, y, z; d = x, y, 1+z; e = x, 1+y, z**

Table S2: Bond Angles of **Complex1**

O1 -Co1 -O2	59.98(11)	O3_d -Co2 -N3	92.15(15)
O1 -Co1 -O5	153.01(12)	O4_d -Co2 -N3	93.23(12)
O1 -Co1 -N1	88.36(12)	N3 -Co2 -C24_d	94.88(13)
O1 -Co1 -C13	29.85(14)	N3 -Co2 -N4_e	176.94(14)
O1 -Co1 -O7_a	89.88(12)	O3_d -Co2 -O8_a	150.28(12)
O1 -Co1 -N2_e	92.28(12)	O4_d -Co2 -O8_a	90.24(13)
O2 -Co1 -O5	93.15(11)	O8_a -Co2 -C24_d	120.74(14)
O2 -Co1 -N1	87.13(11)	O8_a -Co2 -N4_e	86.72(13)

O2 -Co1 -C13	30.16(14)	O3_d -Co2 -O4_d	60.07(13)
O2 -Co1 -O7_a	149.76(11)	O3_d -Co2 -C24_d	29.54(15)
O2 -Co1 -N2_e	92.72(11)	O3_d -Co2 -N4_e	90.91(15)
O5 -Co1 -N1	87.80(13)	O4_d -Co2 -C24_d	30.62(15)
O5 -Co1 -C13	123.19(14)	O4_d -Co2 -N4_e	88.36(12)
O5 -Co1 -O7_a	116.80(12)	N4_e -Co2 -C24_d	87.82(13)
O5 -Co1 -N2_e	91.38(13)	Co1 -O1 -C13	88.0(3)
N1 -Co1 -C13	86.40(13)	Co1 -O2 -C13	91.4(3)
O7_a -Co1 -N1	89.75(12)	Co2_c -O3 -C24	88.3(3)
N1 -Co1 -N2_e	179.16(15)	Co2_c -O4 -C24	90.3(3)
O7_a -Co1 -C13	119.63(14)	Co1 -O5 -C25	120.4(3)
N2_e -Co1 -C13	93.89(13)	Co2 -O6 -C25	151.2(3)
O7_a -Co1 -N2_e	90.80(12)	Co1_f -O7 -C36	173.7(3)
O6 -Co2 -N3	92.01(12)	Co2_f -O8 -C36	119.0(3)
O6 -Co2 -O8_a	122.26(11)	Co1 -N1 -C1	120.8(3)
O3_d -Co2 -O6	87.21(12)	Co1 -N1 -C5	122.7(3)
O4_d -Co2 -O6	147.01(13)	C1 -N1 -C5	116.2(5)
O6 -Co2 -C24_d	116.45(14)	C10 -N2 -C11	115.2(3)
O6 -Co2 -N4_e	88.08(12)	Co1_b -N2 -C10	121.2(3)
O8_a -Co2 -N3	90.65(13)	Co1_b -N2 -C11	123.5(3)
Co2 -N3 -C37	122.1(3)	Co1 -C13 -O1	62.2(3)
Co2 -N3 -C41	121.8(3)	O1 -C13 -C14	120.1(5)
C37 -N3 -C41	115.8(4)	C13 -C14 -C15	118.8(4)
C46 -N4 -C47	115.9(4)	C13 -C14 -C19	120.8(5)
Co2_b -N4 -C46	123.5(3)	C15 -C14 -C19	120.4(4)
Co2_b -N4 -C47	120.2(3)	C14 -C15 -C16	119.4(5)
C52 -N5 -C54	120.00	C15 -C16 -C17	121.5(5)
C59 -N6 -C61	117.3(10)	C18 -C17 -C20	118.4(4)
N1 -C1 -C2	122.7(5)	C16 -C17 -C20	122.2(5)
C1 -C2 -C3	120.7(5)	C16 -C17 -C18	119.4(4)
C2 -C3 -C6	123.9(5)	C17 -C18 -C19	117.4(4)
C2 -C3 -C4	116.2(4)	C17 -C18 -C23	118.7(4)
C4 -C3 -C6	119.9(5)	C19 -C18 -C23	123.9(5)
C3 -C4 -C5	118.8(5)	C14 -C19 -C18	121.9(5)
N1 -C5 -C4	125.3(5)	C17 -C20 -C21	121.6(5)
C3 -C6 -C7	126.3(5)	C20 -C21 -C24	121.6(5)
C6 -C7 -C8	126.4(5)	C22 -C21 -C24	118.4(4)
C7 -C8 -C12	119.7(4)	C20 -C21 -C22	120.0(4)
C9 -C8 -C12	115.4(4)	C21 -C22 -C23	119.6(4)
C7 -C8 -C9	124.9(5)	C18 -C23 -C22	121.7(5)
C8 -C9 -C10	120.6(5)	O3 -C24 -O4	120.9(4)
N2 -C10 -C9	124.0(5)	O4 -C24 -C21	117.8(4)
N2 -C11 -C12	124.9(4)	Co2_c -C24 -O4	59.1(2)
C8 -C12 -C11	119.7(5)	Co2_c -C24 -C21	174.1(3)
Co1 -C13 -C14	174.3(3)	Co2_c -C24 -O3	62.2(3)

O1 -C13 -O2	120.5(4)	O3 -C24 -C21	121.3(5)
Co1 -C13 -O2	58.5(2)	O5 -C25 -C26	117.4(4)
O2 -C13 -C14	119.3(4)	O6 -C25 -C26	118.7(4
O5 -C25 -O6	123.9(4)	N3 -C41 -C40	123.5(5)
C27 -C26 -C31	119.5(4)	C39 -C42 -C43	127.4(6)
C25 -C26 -C31	119.9(4)	C42 -C43 -C44	126.2(6)
C25 -C26 -C27	120.6(4)	C43 -C44 -C45	124.2(5)
C26 -C27 -C28	121.3(4)	C45 -C44 -C48	115.3(5)
C27 -C28 -C35	122.4(4)	C43 -C44 -C48	120.5(5)
C29 -C28 -C35	118.4(4)	C44 -C45 -C46	121.5(5)
C27 -C28 -C29	119.3(4)	N4 -C46 -C45	122.7(5)
C30 -C29 -C32	121.9(4)	N4 -C47 -C48	124.1(5)
C28 -C29 -C30	118.8(4)	C44 -C48 -C47	120.3(5)
C28 -C29 -C32	119.3(4)	N1 -C1 -H1	119.00
C29 -C30 -C31	120.6(4)	C2 -C1 -H1	119.00
C26 -C31 -C30	120.5(4)	C3 -C2 -H2	120.00
C29 -C32 -C33	120.3(4)	C1 -C2 -H2	120.00
C32 -C33 -C36	119.3(4)	C5 -C4 -H4	121.00
C34 -C33 -C36	120.3(4)	C3 -C4 -H4	121.00
C32 -C33 -C34	120.4(4)	C4 -C5 -H5	117.00
C33 -C34 -C35	119.9(4)	N1 -C5 -H5	117.00
C28 -C35 -C34	121.6(4)	C7 -C6 -H6	117.00
O7 -C36 -O8	123.0(5)	C3 -C6 -H6	117.00
O8 -C36 -C33	117.6(4)	C8 -C7 -H7	117.00
O7 -C36 -C33	119.3(4)	C6 -C7 -H7	117.00
N3 -C37 -C38	125.2(5)	C10 -C9 -H9	120.00
C37 -C38 -C39	118.8(5)	C8 -C9 -H9	120.00
C38 -C39 -C42	120.7(5)	N2 -C10 -H10	118.00
C40 -C39 -C42	122.0(5)	C9 -C10 -H10	118.00
C38 -C39 -C40	117.4(5)	N2 -C11 -H11	118.00
C39 -C40 -C41	119.4(5)	C12 -C11 -H11	118.00
C11 -C12 -H12	120.00	C39 -C38 -H38	121.00
C8 -C12 -H12	120.00	C37 -C38 -H38	121.00
C16 -C15 -H15	120.00	C39 -C40 -H40	120.00
C14 -C15 -H15	120.00	C41 -C40 -H40	120.00
C15 -C16 -H16	119.00	C40 -C41 -H41	118.00
C17 -C16 -H16	119.00	N3 -C41 -H41	118.00
C18 -C19 -H19	119.00	C43 -C42 -H42	116.00
C14 -C19 -H19	119.00	C39 -C42 -H42	116.00
C21 -C20 -H20	119.00	C44 -C43 -H43	117.00
C17 -C20 -H20	119.00	C42 -C43 -H43	117.00
C21 -C22 -H22	120.00	C44 -C45 -H45	119.00
C23 -C22 -H22	120.00	C46 -C45 -H45	119.00
C22 -C23 -H23	119.00	C45 -C46 -H46	119.00
C18 -C23 -H23	119.00	N4 -C46 -H46	119.00

C26 -C27 -H27	119.00	N4 -C47 -H47	118.00
C28 -C27 -H27	119.00	C48 -C47 -H47	118.00
C31 -C30 -H30	120.00	C47 -C48 -H48	120.00
C29 -C30 -H30	120.00	C44 -C48 -H48	120.00
C30 -C31 -H31	120.00	C49_g -C49 -C50	119.6(14)
C26 -C31 -H31	120.00	C49 -C50 -C51	127.5(9)
C33 -C32 -H32	120.00	C49 -C50 -C55	112.5(9)
C29 -C32 -H32	120.00	C51 -C50 -C55	119.99
C33 -C34 -H34	120.00	C50 -C51 -C52	119.94
C35 -C34 -H34	120.00	N5 -C52 -C51	120.04
C34 -C35 -H35	119.00	N5 -C54 -C55	120.01
C28 -C35 -H35	119.00	C50 -C55 -C54	120.03
N3 -C37 -H37	117.00	C49_g -C49 -H49	120.00
C38 -C37 -H37	117.00	C50 -C49 -H49	120.00
C50 -C51 -H51	120.00	N6 -C59 -C58	124.7(10)
C52 -C51 -H51	120.00	N6 -C61 -C62	126.5(11)
C51 -C52 -H52	120.00	C57 -C62 -C61	115.9(9)
N5 -C52 -H52	120.00	C57 -C56 -H56	119.00
N5 -C54 -H54	120.00	C56_h -C56 -H56	119.00
C55 -C54 -H54	120.00	C57 -C58 -H58	120.00
C50 -C55 -H55	120.00	C59 -C58 -H58	120.00
C54 -C55 -H55	120.00	N6 -C59 -H59	118.00
C56_h -C56 -C57	122.2(11)	C58 -C59 -H59	118.00
C56 -C57 -C58	130.8(9)	N6 -C61 -H61	117.00
C56 -C57 -C62	113.5(9)	C62 -C61 -H61	117.00
C58 -C57 -C62	115.7(9)	C57 -C62 -H62	122.00
C57 -C58 -C59	119.8(9)	C61 -C62 -H62	122.00

***a = -1+x, y, z; d = x, y, 1+z; e = x, 1+y, z; g = -x, -y, -z; h =1-x, -y, 1-z**

Table S3: π interactions in **complex 1**

π…π interactions				
Cgi – Cgj	Symmetry	π-π(Å)	α	Perpendicular distance of Cgi to Cgj
Cg4-Cg6	x, y, z	3.924(3)	1.5(2)	-3.7493(18)
Cg4-Cg12	x, y, z	4.882(4)	16.8(3)	3.7429(19)
Cg5-Cg7	x, y, z	4.180(3)	25.0(2)	-3.4107(19)
Cg6-Cg4	x, y, z	3.924(3)	1.5(2)	3.778(2)
Cg6-Cg13	x, y, z	4.108(5)	16.4(4)	-3.763(2)
Cg7-Cg5	x, y, z	4.180(3)	25.0(2)	4.0532(18)
Cg8-Cg10	1-x, 1-y, -z	3.759(3)	5.2(2)	3.4949(19)
Cg8-Cg11	1-x, 1-y, -z	3.651(3)	4.1(2)	3.4948(19)
Cg9-Cg11	1-x, 1-y, -z	4.018(3)	5.6(2)	3.4093(19)
Cg10-Cg8	1-x, 1-y, -z	3.759(3)	5.2(2)	3.4232(17)

Cg10-Cg9	1-x, 1-y, -z	4.732(3)	6.6(2)	3.3841(17)
Cg11-Cg8	1-x, 1-y, -z	3.651(3)	4.1(2)	3.5271(17)
Cg11-Cg9	1-x, 1-y, -z	4.018(3)	5.6(2)	3.5438(17)
Cg12-Cg4	x, y, z	4.882(4)	16.8(3)	-4.183(3)
Cg12-Cg13	x, y,-1+z	4.538(6)	13.2(5)	4.500(3)
Cg13-Cg6	x, y, z	4.108(5)	16.4(4)	4.074(4)
Cg13-Cg12	x, y, 1+z	4.538(6)	13.2(5)	-4.272(4)

C-H…π interactions				
C-H…Cg	Symmetry	C…Cg	H…Cg	<C-H…Cg
C31-H31…Cg5	1-x, -y, -z	3.618(5)	2.75	156

***Cg4: N(1)>C(1)>C(2)>C(3)>C(4)>C(5)>; Cg5: N(2)>C(10)>C(9)>C(8)>C(12)>C(11)> ; Cg6: N(3)>C(37)>C(38)>C(39)>C(40)>C(41)>; Cg7: N(4)>C(46)>C(45)>C(44)>C(48)>C(47)> ; Cg8: C(14)>C(15)>C(16)>C(17)>C(18)>C(19)>; Cg9: C(17)>C(18)>C(23)>C(22)>C(21)> C(20)>; Cg10: C(26)>C(27)>C(28)>C(29)>C(30)>C(31)>; Cg11: C(28)>C(29)>C(32)>C(33)>C(34)>C(35)> ; Cg12: N(5)>C(52)>C(51)> C(50)>C(55)>C(54)>; Cg13: N(6)>C(59)>C(58)>C(57)>C(62)>C(61)>**

Table S4: Hydrogen Bond dimensions in **Complex1**

D-H…A	D-H(Å)	H…A(Å)	D…A(Å)	<D-H…A(°)	Symmetry
C1-H1…O5	0.9300	2.4800	3.016(6)	117.00	
C11-H11…O5	0.9300	2.5800	3.116(5)	117.00	x,-1+y,z
C11-H11…O2	0.9300	2.5000	3.101(6)	122.00	1-x,-y,-z
C12-H12…O2	0.9300	2.4100	3.043(6)	125.00	1-x,-y,-z
C19-H19…O2	0.9300	2.4800	2.797(6)	100.00	
C20-H20…O4	0.9300	2.5100	2.817(6)	100.00	
C27-H27…O3	0.9300	2.3600	3.281(6)	169.00	x,y,1+z
C32-H32…O1	0.9300	2.5000	3.421(6)	169.00	1+x,y,z
C41-H41…O8	0.9300	2.5300	3.047(6)	115.00	-1+x,y,z
C46-H46…O6	0.9300	2.4600	3.005(6)	117.00	x,-1+y,z
C47-H47….O8	0.9300	2.5800	3.049(6)	112.00	-1+x,y,z
C48-H48…O4	0.9300	2.4200	3.233(6)	147.00	-x,-y,-z

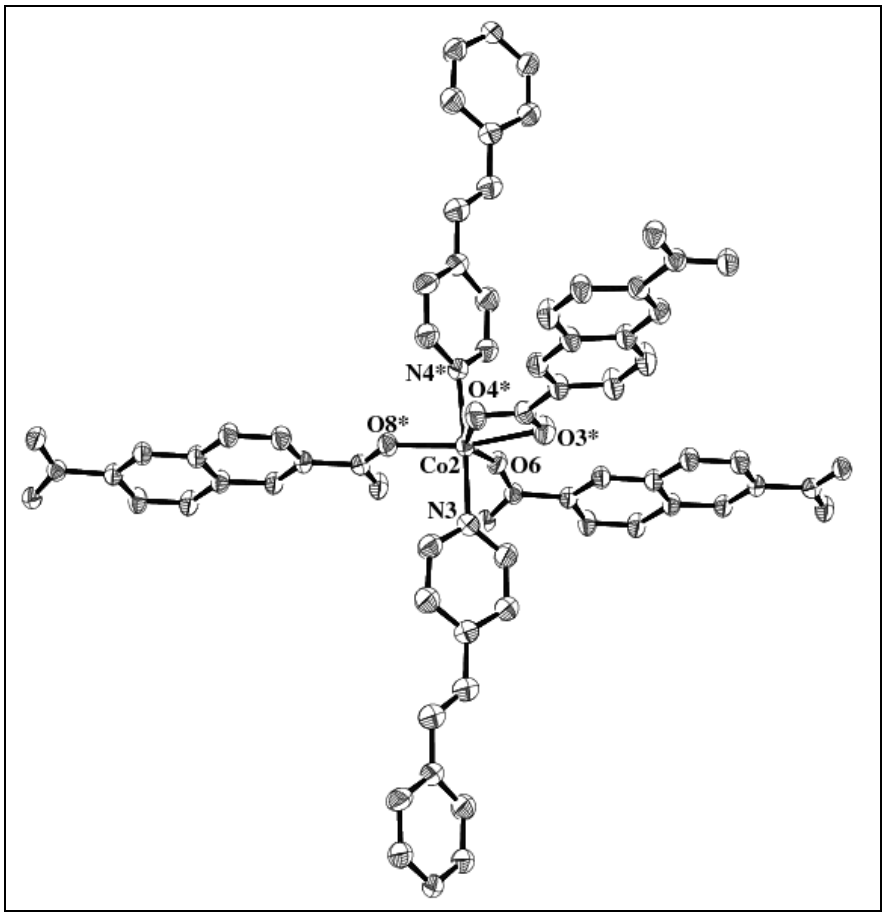

Figure S1: The ORTEP diagram of **complex 1** (30 % atomic probability)

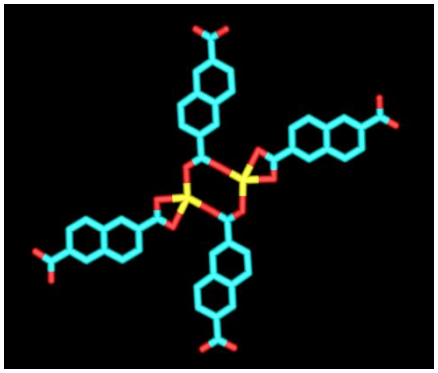

Figure S2: $[Co_2(COO)_4]_n$ Paddle-wheel like SBU

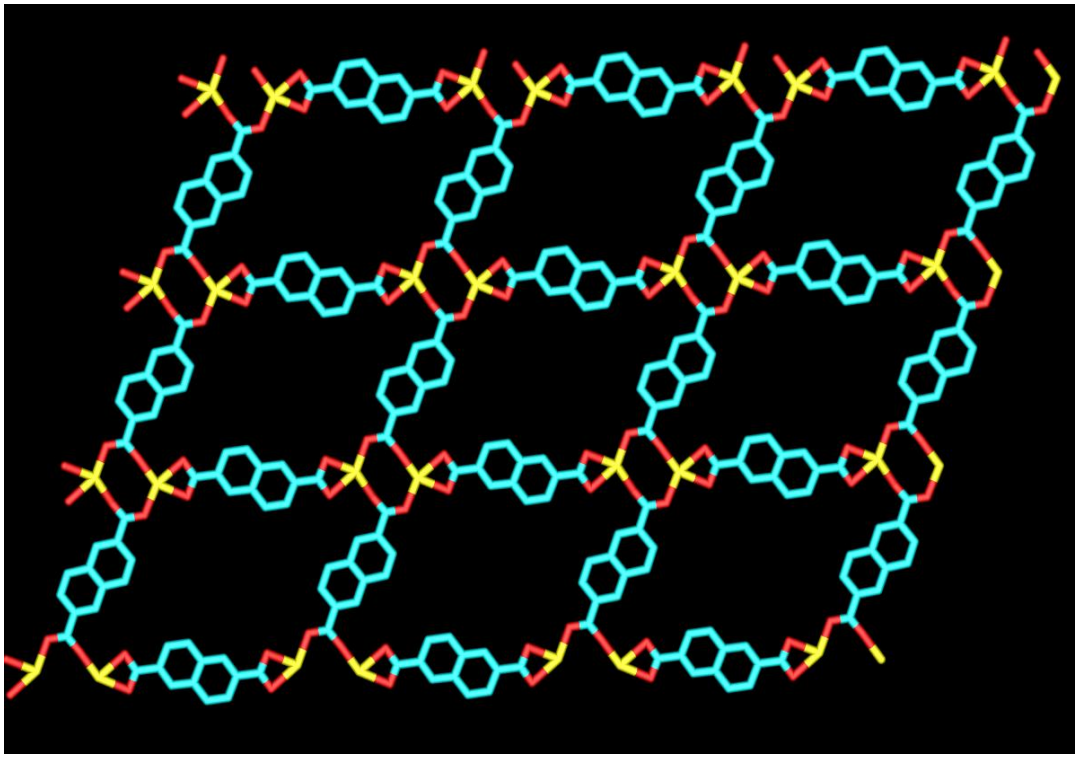

Figure S3: The 2D coordination sheet formed by connecting SBU's $[Co_2(COO)_4]_n$ with ndc^{2-} ligands

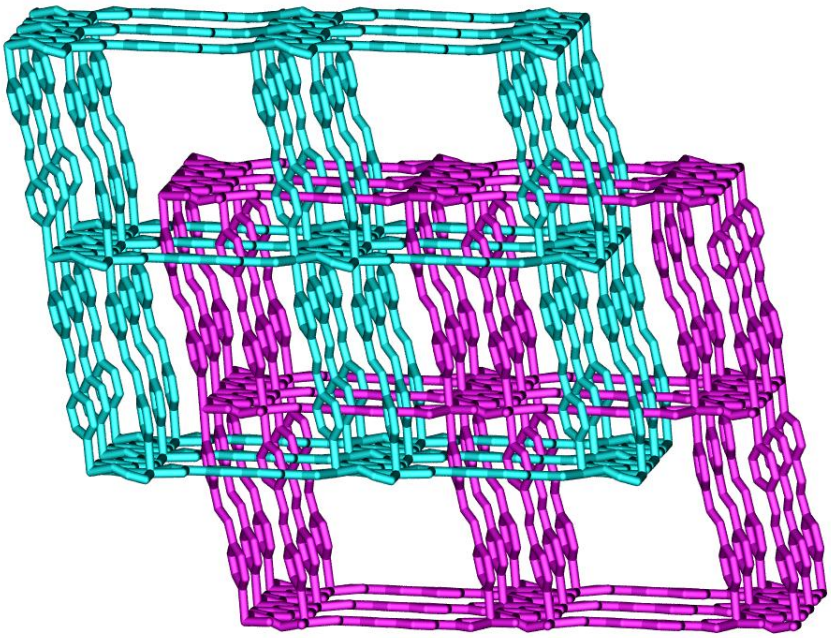

Figure S4: 2 fold self-catenated framework

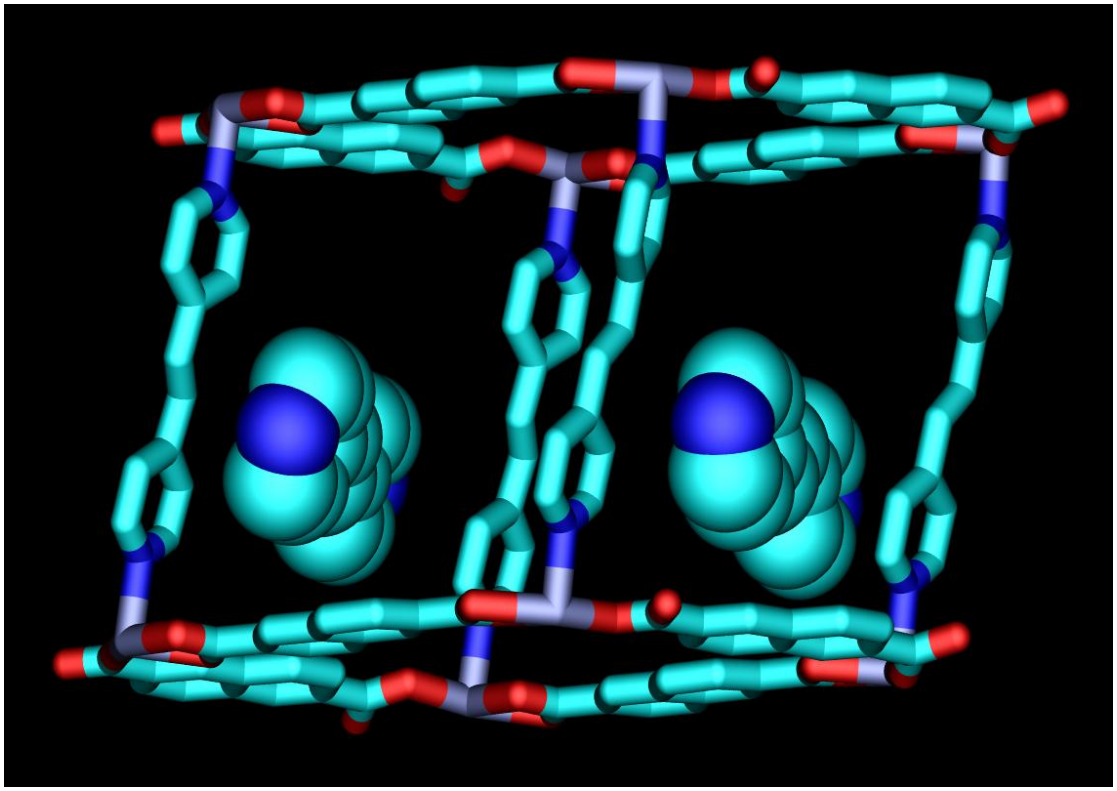

Figure S5: The guest bpee molecules are in the voids

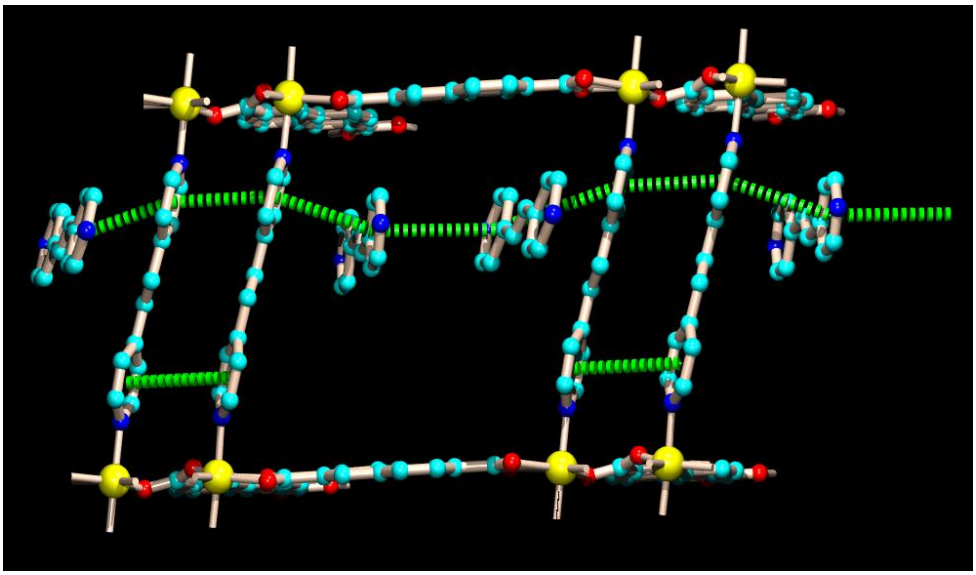

Figure S6: The guest bpee molecules are attached to the host through π…π interactions

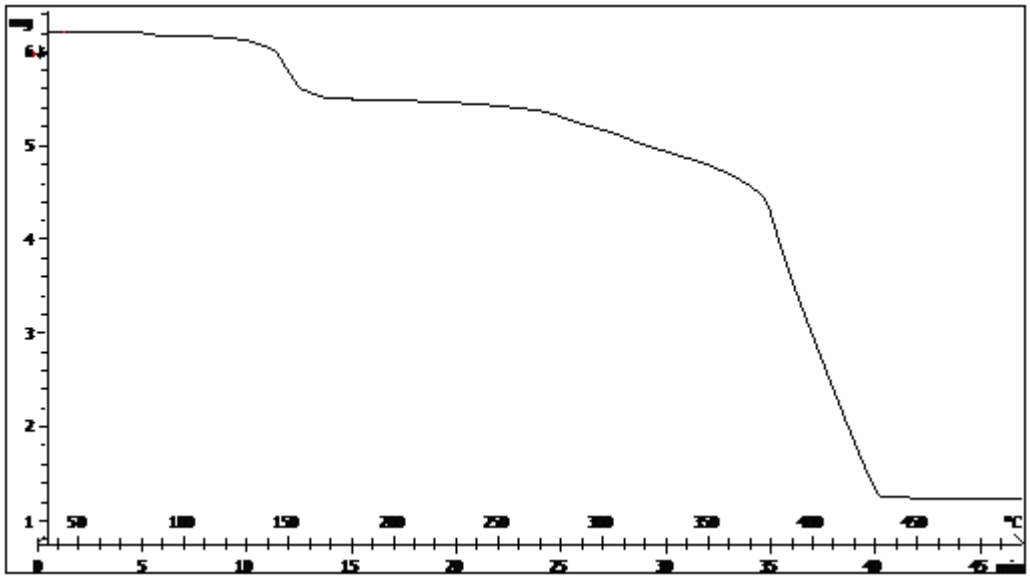

Figure S7: Thermal plot of the **complex 1**

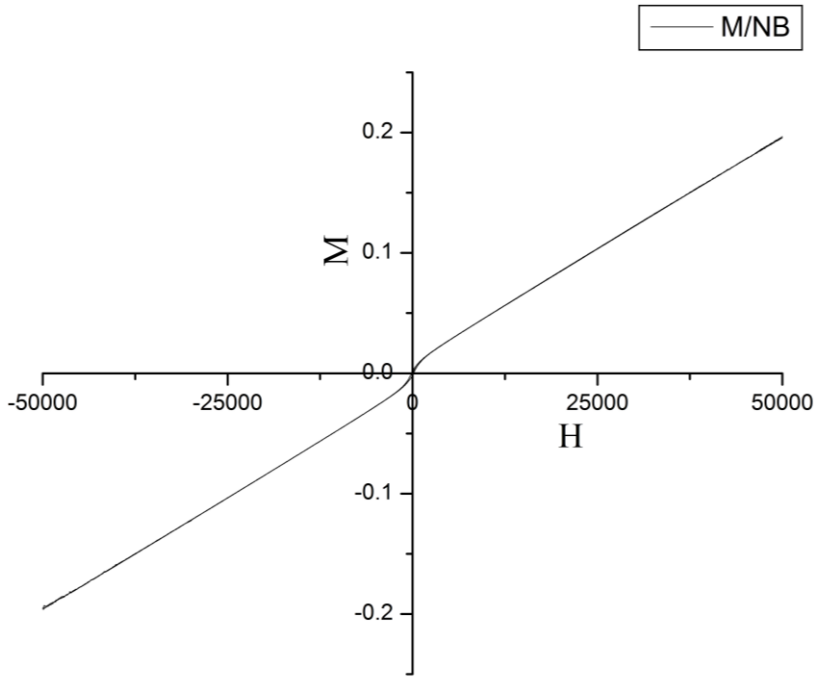

Figure S8: M*vs*H loop of **complex 1** upto 50000Oe

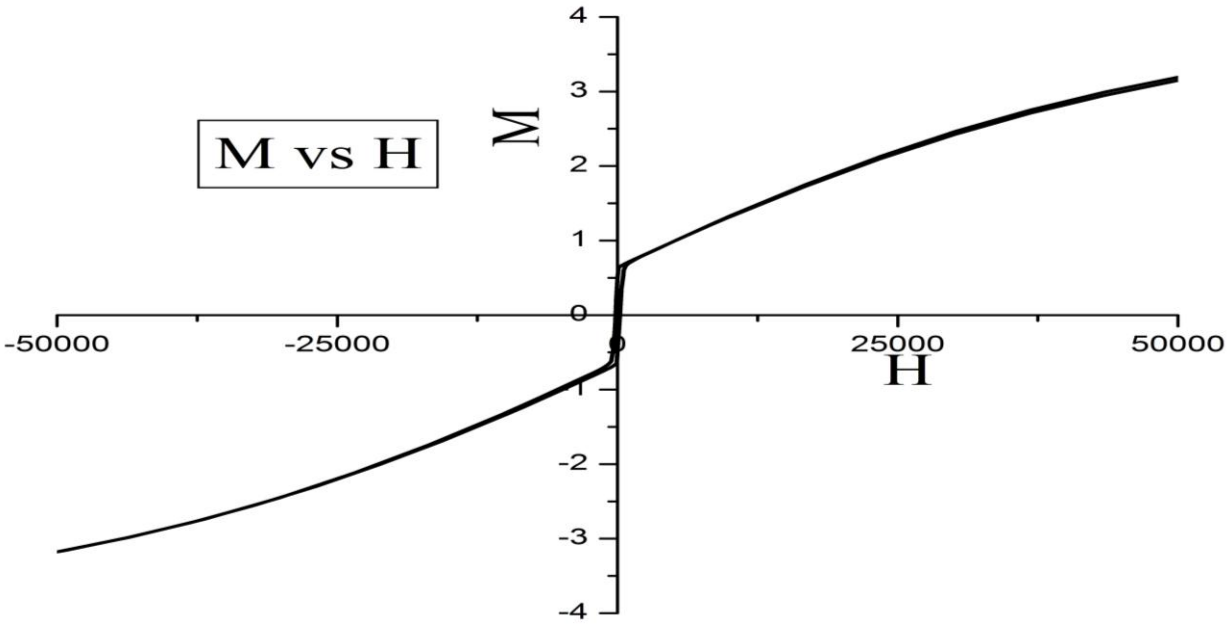

Figure S9: M*vs*H loop of the evacuated framework upto 50000Oe

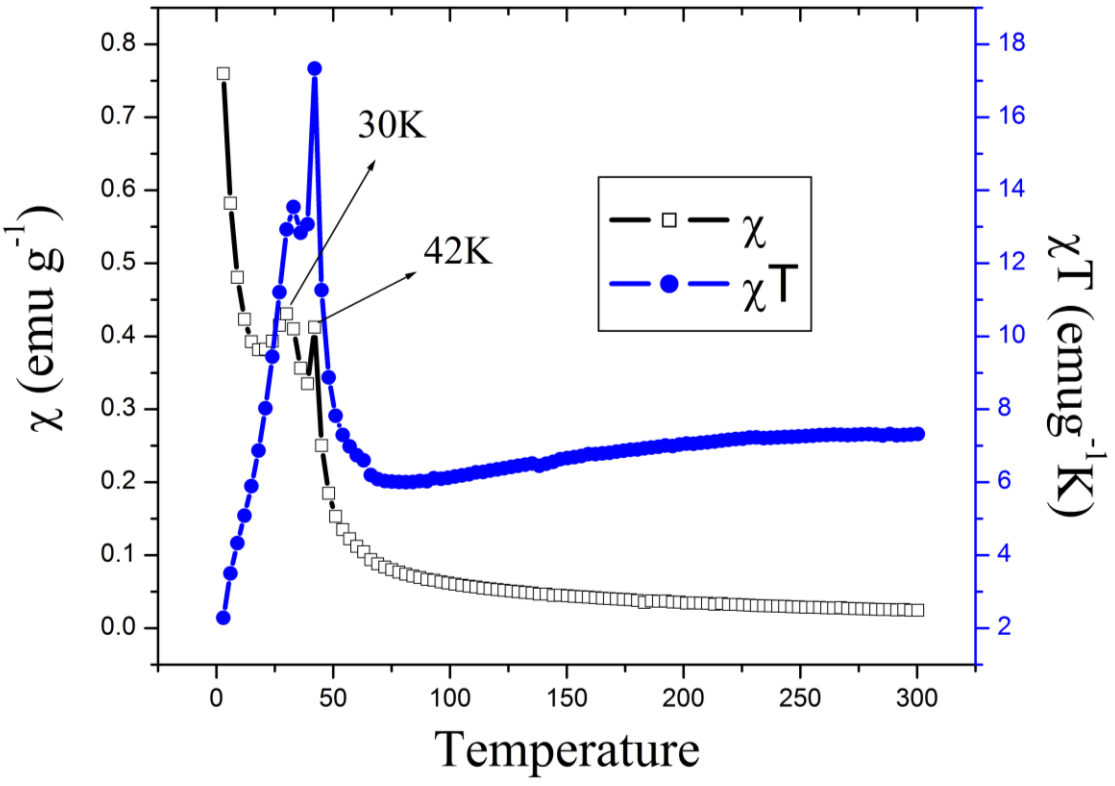

Figure 10: χ*vs*T and χT*vs*T plot of complex after reabsorption of guest

(In absence of proper structural data molecular weight can't be estimated, we therefore represent the magnetic data in emu unit)

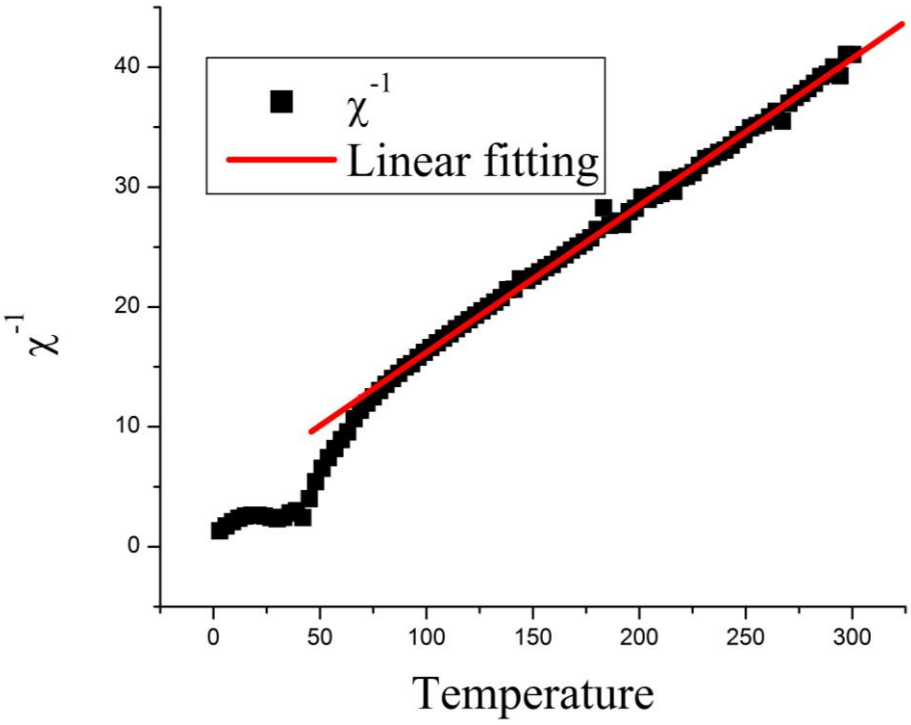

Figure S11: χ^{-1}*vs*T plot of the complex after reabsorption of guest

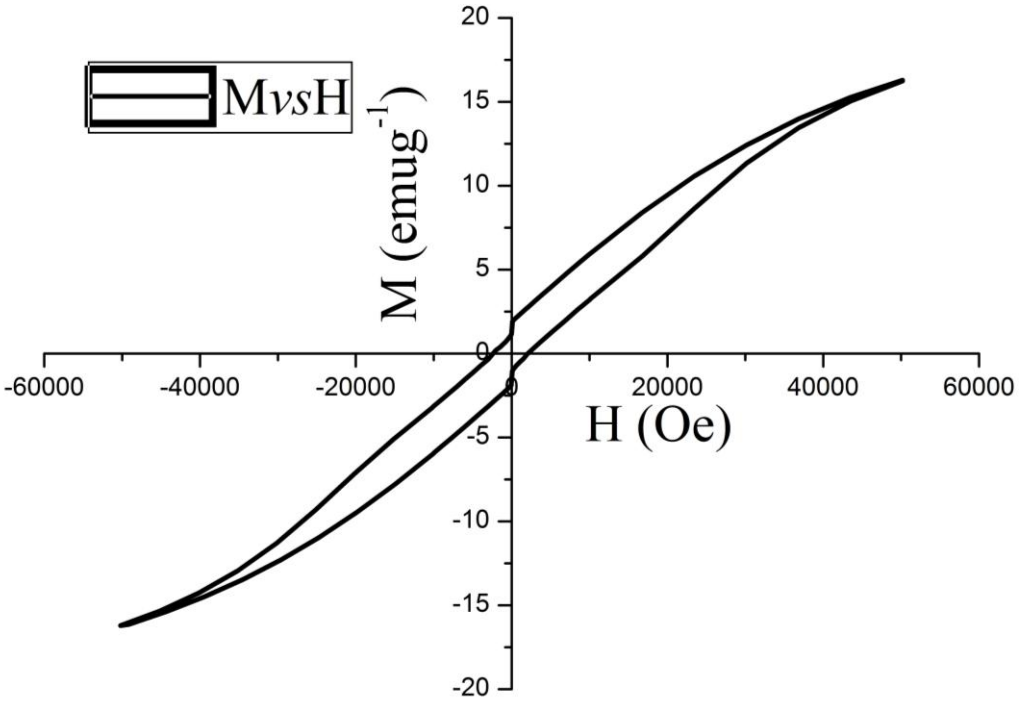

Figure S12: M*vs*H plot of the complex after reabsorption