Supporting information for

Auxiliary ligand aided tuning of aggregation in transition metal benzoates: Isolation of four different types of coordination polymers

Subarna Banerjee,[a] Palanisamy Rajakannu,[a] Ray. J. Butcher,[b] and Ramaswamy Murugavel*[a]

[a]*Department of Chemistry, Indian Institute of Technology Bombay, Powai, Mumbai 400 017, India. E-mail address: rmv@chem.iitb.ac.in; Tel: +91 22 2576 7163; Fax: +91 22 2572 3480/2576 7152.* [b] *Department of Chemistry, Howard University, Washington, DC 20059, USA.*

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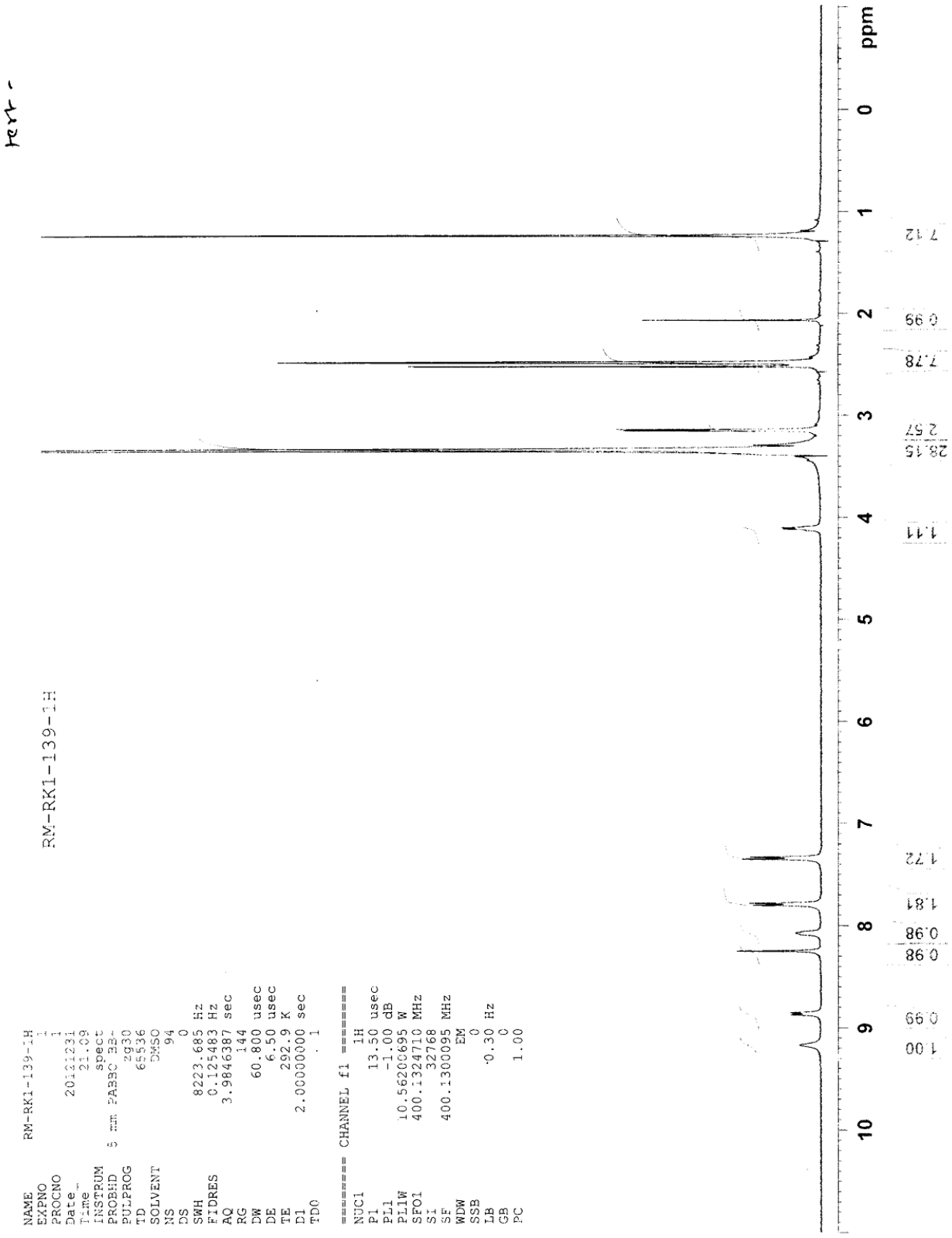


Fig. S1. ^{1}H NMR spectrum of **3** in DMSO-d_6.

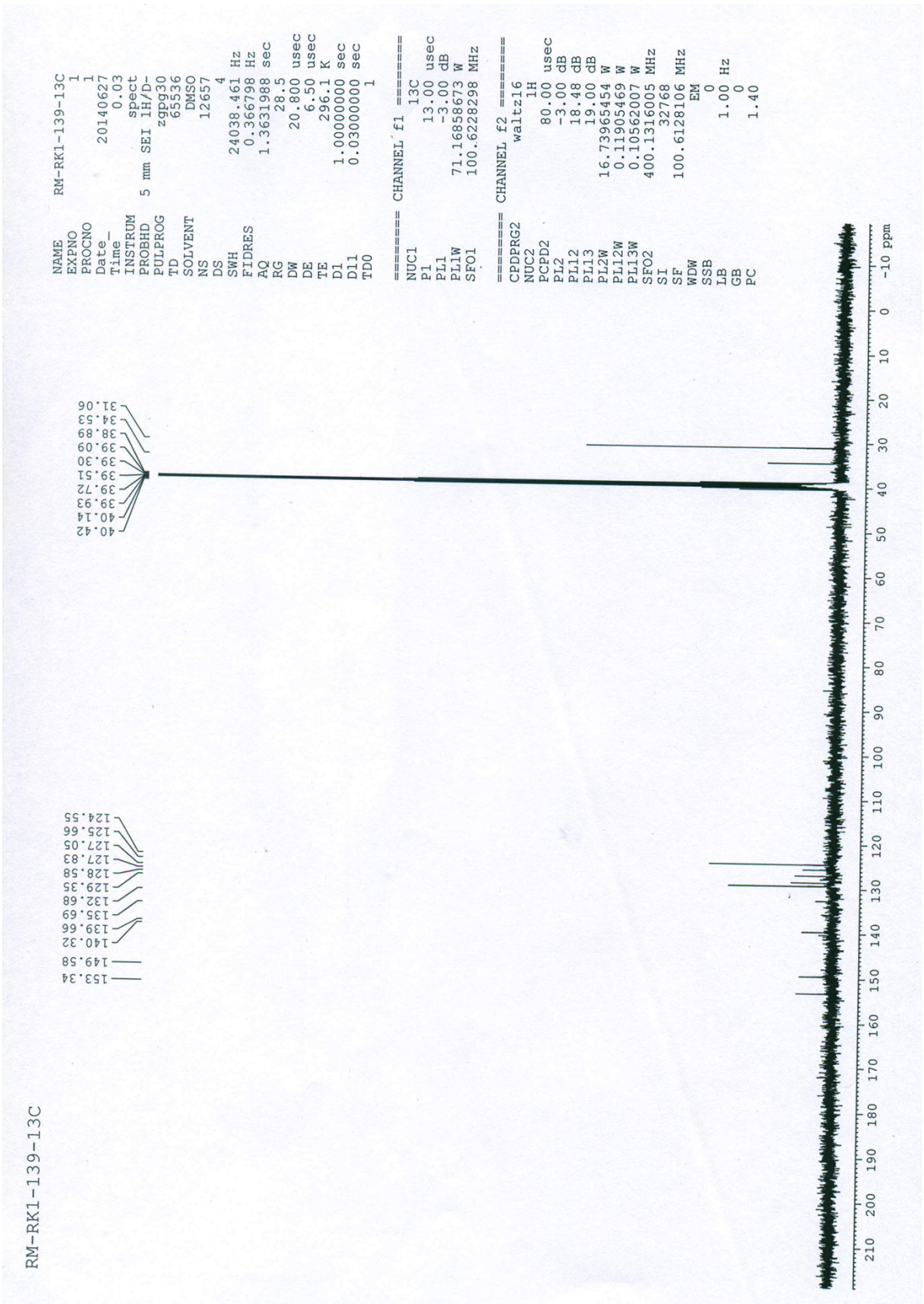


Fig. S2. ^{13}C NMR spectrum of **3** in DMSO-d_6.

Fig. S3. ^{1}H NMR spectrum of **7** in DMSO-d_6.

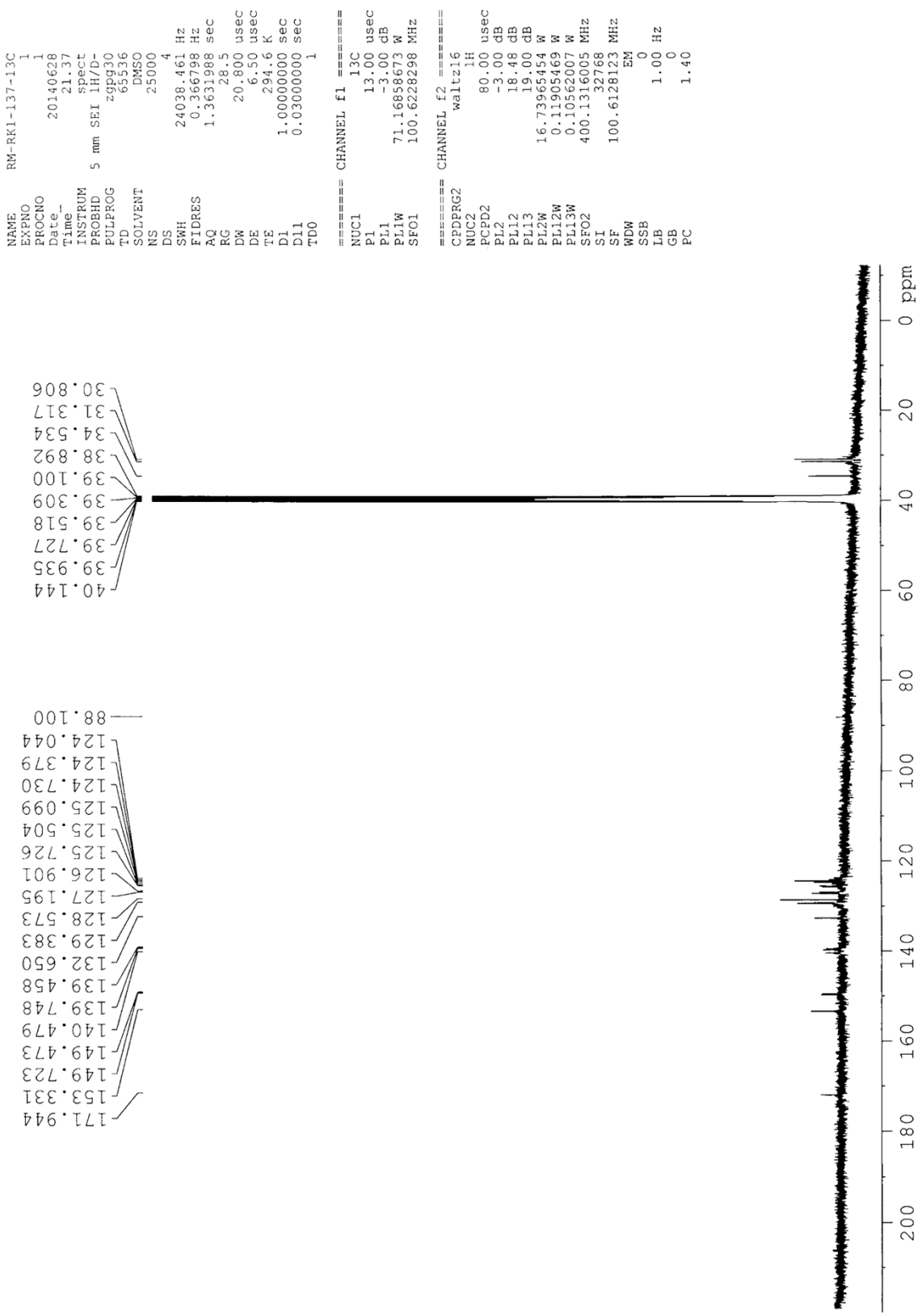


Fig. S4. ^{13}C NMR spectrum of **7** in DMSO-d_6.

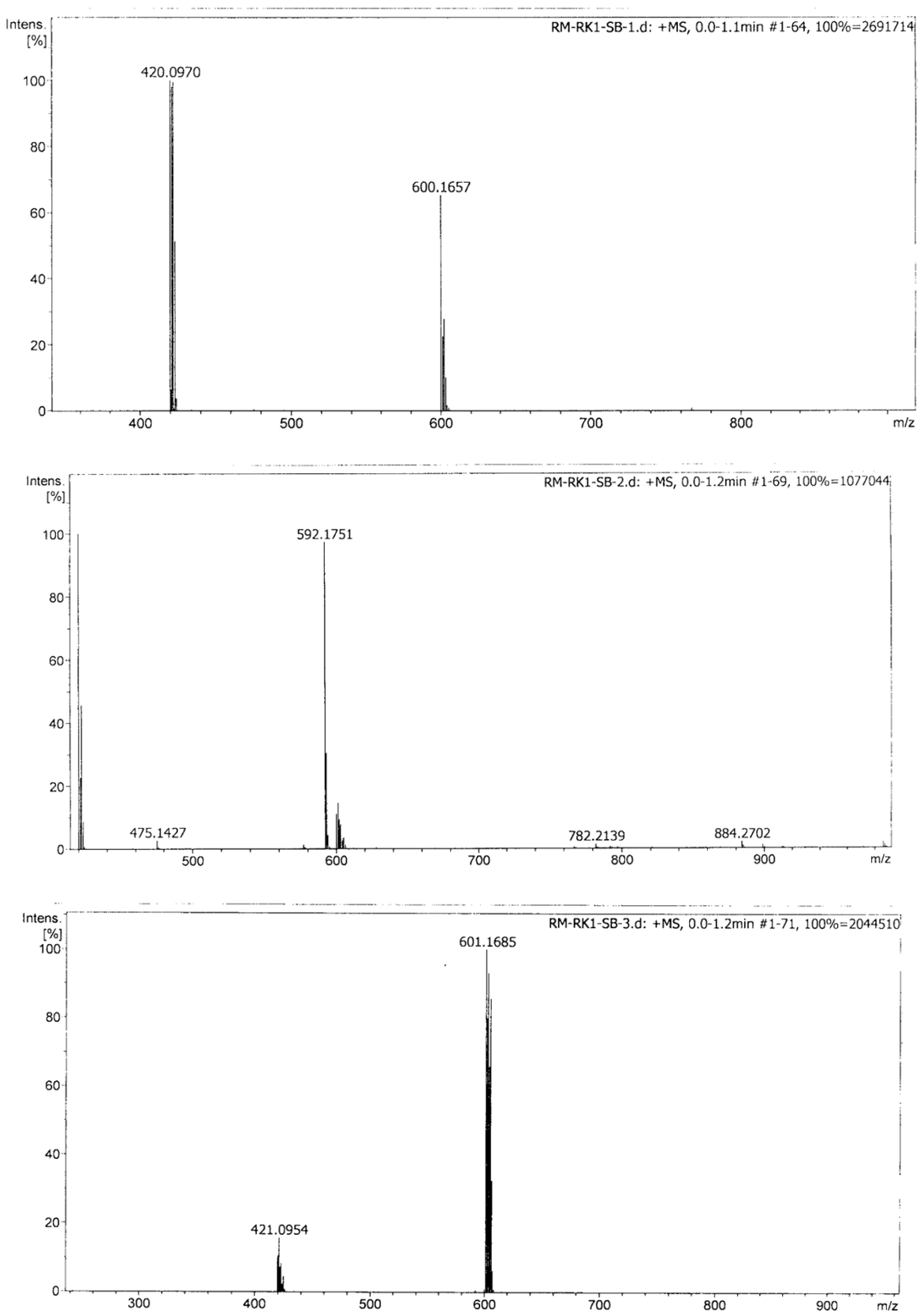


Fig. S5. ESI-MS spectra of **1-3** (from top to bottom) in DMSO+CH_3OH mixture.

Table S1. Selected structural parameters observed in $[Cu(L^1)_2(AL^1)(H_2O)](H_2O)$ (**1**).

Bond lengths (Å)			
Cu(1)–O(1)	1.928(2)	O(1)–C(1)	1.279(4)
Cu(1)–O(3)	1.948(2)	O(2)–C(1)	1.231(4)
Cu(1)–N(1)	2.013(3)	O(3)–C(12)	1.275(4)
Cu(1)–N(2)	2.033(3)	O(4)–C(12)	1.229(4)
Cu(1)–O(5)	2.296(3)	O(5)–H(5A)	0.71(4)
N(1)–C(23)	1.328(5)	O(5)–H(5B)	0.81(6)
Bond angles (°)			
O(1)–Cu(1)–O(3)	90.2(1)	C(27)–N(1)–Cu(1)	113.6(2)
O(1)–Cu(1)–N(1)	169.0(1)	C(34)–N(2)–C(31)	117.9(3)
O(3)–Cu(1)–N(1)	92.0(1)	C(34)–N(2)–Cu(1)	129.3(2)
O(1)–Cu(1)–N(2)	91.9(1)	C(31)–N(2)–Cu(1)	112.7(2)
O(3)–Cu(1)–N(2)	152.1(1)	C(1)–O(1)–Cu(1)	127.9(2)
N(1)–Cu(1)–N(2)	81.2(1)	C(12)–O(3)–Cu(1)	128.2(2)
O(1)–Cu(1)–O(5)	97.5(1)	Cu(1)–O(5)–H(5A)	94(4)
O(3)–Cu(1)–O(5)	98.3(1)	Cu(1)–O(5)–H(5B)	87(4)
N(1)–Cu(1)–O(5)	92.9(1)	H(5A)–O(5)–H(5B)	120(5)
N(2)–Cu(1)–O(5)	108.9(1)	H(6A)–O(6)–H(6B)	109(4)

Table S2 Comparison of copper-phenanthroline complexes with –O and –N coordination.

Compound	Geometry around Cu	Cu–O (carboxy) (Å)	Cu–N (hc)* (Å)	Cu–O (aqua) (Å)	<N–Cu–N (°)	Nature of COO^-	Type of structure	Ref.*
$[Cu(L^3)_2(AL^1)(H_2O)]$ (**4**)	distorted O_h	1.947(5)	2.015(5), 2.027(5)	2.005(5)	81.5(2)	monodentate	3-D network	this work
$[CuCl(phen)(C_8H_4NO_2)(H_2O)]\cdot H_2O$ [a]	sq. pyramidal	1.976(2)	–	–	–	monodentate	1–D network	17a
$[CuCl(phen)(C_7H_7O_3S)(H_2O)]$ [b]	distorted sq. pyramidal	–	2.006(3), 2.028(3)	1.984(3)	81.2(1)	–	Supra molecular	17b
$[Cu(HCO_3)(phen)_2]ClO_4$	tetragonal pyramidal	1.998(11)	2.05(1), 1.987(11), 1.988(11), 2.17(1)	–	82.2(3), 80.9(3)	monodentate	–	17c
$[Cu(HCO_3)(phen)_2]ClO_4$	distorted TBP	2.359(3)	1.997(2), 2.119(2)	–	80.68(8)	bidentate	–	17c
[Cu(phen)(L-asp)$(H_2O)]4H_2O$ [c]	elongated rhombic O_h	2.560(3)	2.020, 1.994	2.446(3)	82.0(1)	monodentate	–	17d
Glycylglycinato(phen) Cu^{II}trihydrate	distorted sq. pyramidal	2.008(4)	2.009(5), 2.275(5)	–	78.3(2)	monodentate	polymeri-c lattice	17e
[Cu(pAB)$(phen)(H_2O)]_2(NO_3)_2\cdot 2pABH\cdot 2H_2O$ [d]	distorted O_h	1.946(4), 1.936(4)	2.012(5), 2.019(5)	2.272(5)	82.1(3)	bidentate	dimeric	17f
$[Cu(phen)(ox)(H_2O)]$ [e]	distorted sq. pyramidal	1.937(2), 1.944(2)	2.005(2), 2.011(2)	2.221(2)	82.3(1)	monodentate	3-D	17g

*hc: heterocyclic; [a] $C_8H_4NO_2$: 4-cyanobenzoate; [b] $C_7H_7O_3S$: p-toluene sulfonate; [c] L-asp: L-aspartate; [d] pAB: 4-aminobenzoate; pABH: 4-aminobenzoic acid; [e] ox: oxalate; [f] sal: salicylate; [g] $bdoaH_2$: benzene-1,2-dioxyacetic acid; [h] mal: malonate.

* References are included in main text.

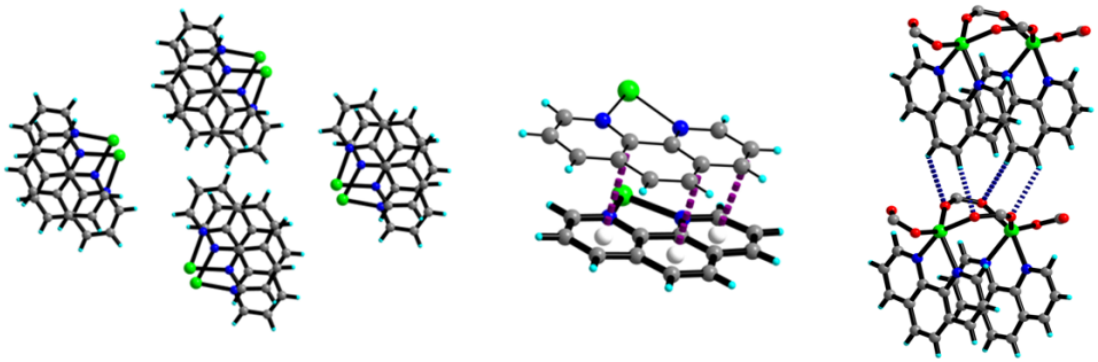


Fig. S6 π-π interactions and CH-π interactions in **1**.

Table S3 Selected structural parameters observed in $[Mn_2(L^1)_4(AL^1)_2](CH_3OH)$ (**2**).

Bond lengths (Å)			
N(1)-Mn(01)	2.273(7)	C(16)-N(1)	1.364(6)
N(2)-Mn(01)	2.296(7)	C(20)-N(2)	1.356(5)
O(2)-Mn(01)	2.114(8)	C(23)-N(2)	1.330(6)
O(3)-Mn(01)	2.062(8)	C(7)-O(1)	1.240(7)
O(4)-Mn(01)	2.126(6)	C(7)-O(2)	1.269(6)
C(12)-N(1)	1.330(6)	C(30)-O(3)	1.260(6)
Bond angles (°)			
C(12)-N(1)-Mn(01)	125.5(3)	O(3)-Mn(01)-O(2)	137.1(2)
C(16)-N(1)-Mn(01)	116.8(3)	O(3)-Mn(01)-O(4)	96.6(2)
C(23)-N(2)-C(20)	117.9(3)	O(2)-Mn(01)-O(4)	87.8(3)
C(23)-N(2)-Mn(01)	125.6(2)	O(3)-Mn(01)-N(1)	86.9(3)
C(20)-N(2)-Mn(01)	115.8(3)	O(2)-Mn(01)-N(1)	105.1(2)
C(7)-O(2)-Mn(01)	100.9(3)	O(4)-Mn(01)-N(1)	156.92(9)
C(30)-O(3)-Mn(01)	154.4(2)	O(3)-Mn(01)-N(2)	130.78(13)

Table S4. Comparison of manganese-phenanthroline complexes with –O and –N coordination with **2** and **4**.

Compound	A	Mn–O (carboxy) (Å)	Mn–N (hc)* (Å)	Mn–O (aqua) (Å)	N···N (Å)	N-Mn-N (°)	nature of COO^-	Str. type	Ref.*
$[Mn_2(L^1)_4(AL^1)_2](CH_3OH)$ (**2**)	*4	2.126, 2.114, 2.062	2.297, 2.274	-	2.701	72.44	Mono & bidentate	Dimeric	this work
$[Mn(L^3)_2(AL^1)(H_2O)]$ (**4**)	*1	2.099(1)	2.247(1), 2.244(1)	2.220(1)	2.716	74.43(5)	#1	3-D	this work
$[Mn(PhCOO)(phen)_2(H_2O)](ClO_4)(dmf)$[a]	*1	2.124(3)	2.261(3), 2.303(3)	2.156(3)	2.702(1), 2.709(2)	73.3(1)-72.4(1)	#1	–	18a
$\{[Mn(5\text{-}HIA)(phen)]H_2O\}_n$[b]	*1	–	–	–	–	–	#2	Polymeric chain	18b
$[Mn(ClCH_2COO)(phen)_2(H_2O)]ClO_4$	*2	2.119(3)	2.243(3), 2.375(4)	2.182(3)	2.700(3), 2.692(3)	71.4(1),73.1(1)	#1	Dimeric	18c
$[Mn_2(C_4H_4O_4)_2(phen)_2(H_2O)_4]2H_2O$[c]	*1	2.123(2),2.180(2)	2.307(2), 2.308(2)	2.265(2)-2.243(2)	–	72.05(6)	#3	2-D layer	18d
$[Mn(phen)_2(H_2O)_2](fum)(4H_2O)$[d]	*3	–	2.269(1), 2.273(1)	2.130(1), 2.143(1)	–	73.22(4)	–	–	18e
$[Mn(phen)(bet)(NO_3)(H_2O)_2](NO_3)(H_2O)$[e]	*1	2.194(4)	2.275(3), 2.302(4)	2.190(3), 2.195(3)	–	72.4(1)	#1	Monomeric species	18f
$[Mn_2(phen)_4(ta)(H_2O)_2](ClO_4))_2$[f]	*1	2.120(3)	2.291(4), 2.256(4), 2.272(4), 2.281(4)	2.141(4)	–	73.0(2)	#3	–	18g

A: geometry around Mn; *hc: heterocyclic; [a] dmf: dimethylformamide; [b] HIA: 5-hydroxy-isophthalic acid (the acid is dianionic in the compound); [c] $(C_4H_4O_4)^{2-}$: succinate anion; [d] $fumH_2$: fumaric acid; [e] bet: betaine ($Me_3N^+CH2CO2^-$); [f] ta: terephthalate; *1 distorted O_h; *2 severly distorted O_h; *3 O_h; *4 square pyramidal; #1 monodentate; #2 chelating; #3 bismonodentate.

* References are included in main text.

Table S5. Selected structural parameters observed in $[Zn_2(L^1)_4(AL^1)_2](CH_3OH)$ (**3**).

Bond lengths (Å)			
N(1)-Zn(01)	2.165(4)	C(17)-O(3)	1.252(5)
N(2)-Zn(01)	2.167(4)	C(17)-O(4)#1	1.255(5)
O(2)-Zn(01)	1.962(4)	C(22)-N(1)	1.333(5)
O(4)-Zn(01)	2.042(4)	C(31)-N(2)	1.329(5)
C(10)-O(1)	1.221(5)	C(33)-N(2)	1.360(5)
C(10)-O(2)	1.294(5)	C(34)-N(1)	1.353(5)
Bond angles (°)			
C(22)-N(1)-Zn(01)	126.9(3)	O(2)-Zn(01)-O(3)	117.13(17)
C(34)-N(1)-Zn(01)	115.0(3)	O(2)-Zn(01)-O(4)	91.86(19)
C(31)-N(2)-C(33)	118.5(3)	O(3)-Zn(01)-O(4)	96.24(15)
C(31)-N(2)-Zn(01)	126.9(3)	O(2)-Zn(01)-N(1)	103.02(17)
C(33)-N(2)-Zn(01)	114.4(3)	O(3)-Zn(01)-N(1)	88.51(18)
C(10)-O(2)-Zn(01)	117.0(3)	O(4)-Zn(01)-N(1)	160.28(11)
C(17)-O(3)-Zn(01)	146.3(3)	O(2)-Zn(01)-N(2)	102.20(16)
Hydrogen bonds			
D–H···A (Å)	D–H (Å)	H···A (Å)	D···A (Å)
O5–H5A···O2[a]	0.76(3)	1.96(3)	2.688(2)
O5–H5B···O3[b]	0.82(2)	2.02(2)	2.822(2)

Table S6. Comparison of zinc-phenanthroline complexes with –O and –N coordination with **3** and **7**.

Compound	Geom. around Zn	Zn–O (COO^-)(Å)	Zn–N (hc)*(Å)	Zn–O (aqua) (Å)	<N–Zn–N (°)	Nature of COO^-	Str. type	Ref.*
$[Zn_2(L^1)_4(AL^1)_2](CH_3OH)$ (**3**)	square pyramidal	1.962(4) 2.042(4)	2.165(4) 2.167(4)	–	76.34(19)	Mono & bidentate	Dimeric	This work
$[Zn(L^3)_2(AL^1)(H_2O)]$ (**7**)	dist. O_h	–	–	–	–	mono-dentate	3-D	this work
$[Zn(phen)_2(H_2O)_2]L\cdot 4H_2O$[a]	O_h	–	2.152(2), 2.232(2)	2.074(1) 2.049(1)	76.09(6)	–	3-D	19a
$[Zn(phen)_2(MeCO_2)]ClO_4$	dist. O_h	2.296(5) 2.156(5)	2.143(6), 2.135(6), 2.100(5), 2.160(5)	-	78.1(2), 78.6(2)	bi-dentate	–	19b

*hc: heterocyclic; [a] L^{2-}= fumarate

* References are included in main text.

Table S7. Selected structural parameters observed in $[Mn(L^3)_2(AL^1)(H_2O)]$ (**4**).

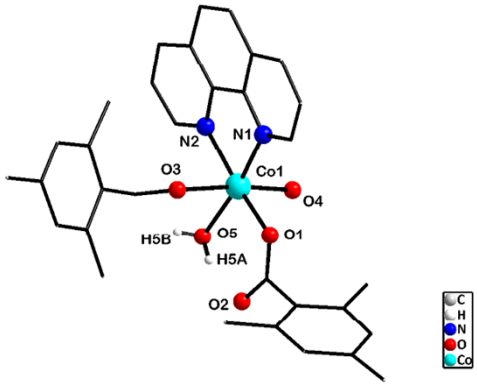
Bond lengths (Å)			
Mn(1)–O(1)	2.099(1)	O(1)–C(1)	1.263(2)
Mn(1)–O(3)	2.189(1)	O(2)–C(1)	1.243(2)
Mn(1)–O(5)	2.220(1)	O(3)–C(11)	1.269(2)
Mn(1)–N(2)	2.244(1)	O(4)–C(11)#1	1.250(2)
Mn(1)–N(1)	2.247(1)	O(5)–H(5A)	0.76(3)
Mn(1)–O(4)	2.251(1)	O(5)–H(5B)	0.82(3)
Bond angles (°)			
O(1)–Mn(1)–O(3)	93.41(5)	O(3)–Mn(1)–O(4)	171.30(4)
O(1)–Mn(1)–O(5)	95.98(5)	O(5)–Mn(1)–O(4)	3.24(5)
O(3)–Mn(1)–O(5)	88.23(5)	N(2)–Mn(1)–O(4)	5.37(4)
O(1)–Mn(1)–N(2)	89.12(5)	N(1)–Mn(1)–O(4)	81.95(5)
O(3)–Mn(1)–N(2)	102.96(5)	C(1)–O(1)–Mn(1)	126.2(1)
O(5)–Mn(1)–N(2)	167.44(5)	C(11)–O(3)–Mn(1)	136.3(1)
O(1)–Mn(1)–N(1)	161.83(5)	C(11)#1–O(4)–Mn(1)	131.5(1)
O(3)–Mn(1)–N(1)	97.71(5)	Mn(1)–O(5)–H(5A)	97(2)
O(5)–Mn(1)–N(1)	98.67(5)	Mn(1)–O(5)–H(5B)	98(2)

Symmetry equivalents: #1 y, -x+1/2, z+1/4; #2 -y+1/2, x, z-1/4 (a) x,y,z (b) y, x+1/2, +z+1/4

Table S8. Selected structural parameters observed in $[Cu(L^3)_2(AL^1)(H_2O)]$ (**6**).

Bond lengths (Å)			
Cu(1)–O(1)	1.947(5)	O(1)–C(1)	1.261(9)
Cu(1)–O(5)	2.005(5)	O(2)–C(1)	1.238(9)
Cu(1)–N(1)	2.015(5)	O(3)–C(11)	1.249(8)
Cu(1)–N(2)	2.027(5)	O(4)–C(11)	1.272(8)
Cu(1)–O(3)	2.405(5)		
Bond angles (°)			
O(1)–Cu(1)–O(5)	96.0(2)	N(2)–Cu(1)–O(3)	86.9(2)
O(1)–Cu(1)–N(1)	170.7(2)	C(21)–N(1)–Cu(1)	129.0(5)
O(5)–Cu(1)–N(1)	92.2(2)	C(25)–N(1)–Cu(1)	112.4(5)
O(1)–Cu(1)–N(2)	89.8(2)	C(32)–N(2)–Cu(1)	128.6(5)
O(5)–Cu(1)–N(2)	170.9(3)	C(29)–N(2)–Cu(1)	112.6(5)
N(1)–Cu(1)–N(2)	81.5(2)	C(1)–O(1)–Cu(1)	128.4(5)
O(1)–Cu(1)–O(3)	88.9(2)	C(11)–O(3)–Cu(1)	123.5(4)
O(5)–Cu(1)–O(3)	86.2(2)	Cu(1)–O(5)–H(5A)	101(4)
N(1)–Cu(1)–O(3)	87.3(2)	Cu(1)–O(5)–H(5B)	105(4)

(a)



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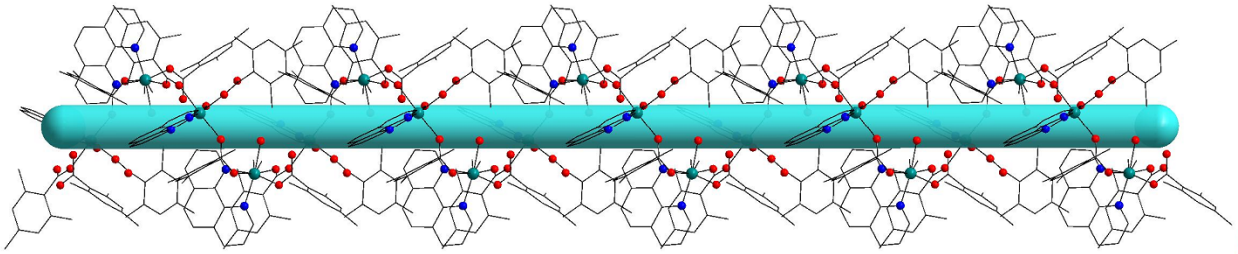

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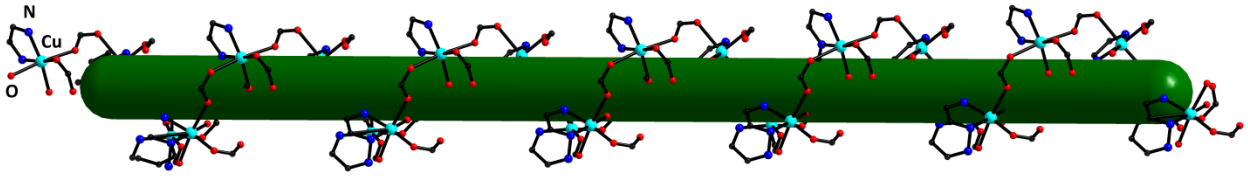

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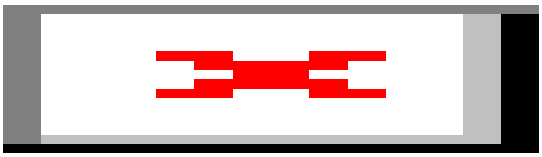

Fig. S7 Molecular structure of **5**(a) and helical structure of [Co(tmba)$_2$(1,10-phen)(H$_2$O)] (**5**, b) [Cu(tmba)$_2$(1,10-phen)(H$_2$O)] (**6**, c) and [Zn(tmba)$_2$(1,10-phen)(H$_2$O)] (**7**, d).

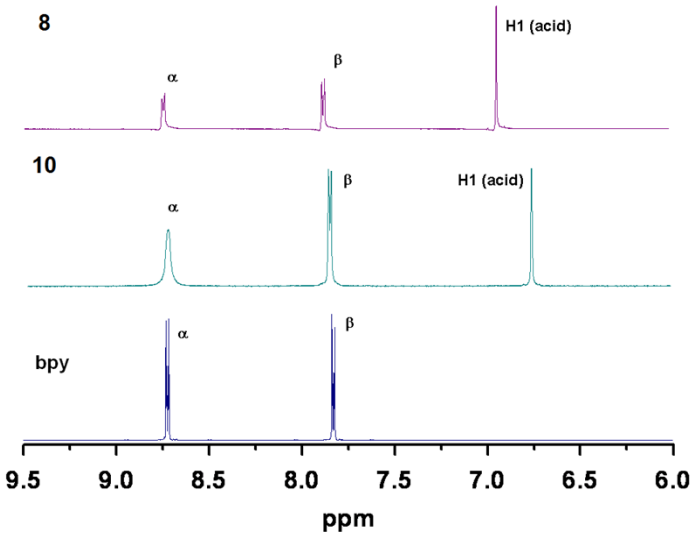

Fig. S8 ^{1}H NMR spectra of **8** (top) and **10** (middle) with free 4,4'-bpy (bottom) ligand in DMSO-d_6.

Table S9. Selected bond length and angles of $[Zn(L^2)_2(AL^2)]$ (**8**).

Bond lengths (Å)			
Zn(1)–N(1)	2.130(2)	O(1)–C(1)	1.265(4)
Zn(1)–O(2)	2.136(2)	O(2)–C(1)	1.260(4)
Zn(1)–O(1)	2.162(2)	N(1)–C(21)	1.325(3)
Bond angles (°)			
N(1)#1–Zn(1)–N(1)	180.0	O(1)#1–Zn(1)–O(1)	180.0
N(1)–Zn(1)–O(2)#1	90.0	C(1)–O(1)–Zn(1)	88.1(2)
N(1)–Zn(1)–O(2)	90.0	C(1)–O(2)–Zn(1)	89.4(2)
O(2)#1–Zn(1)–O(2)	180.0	C(21)#2–N(1)–C(21)	116.7(3)
N(1)–Zn(1)–O(1)#1	90.0	C(21)#2–N(1)–Zn(1)	121.7(1)
N(1)#1–Zn(1) –O(1)	90.0	C(21)–N(1)–Zn(1)	121.7(1)
N(1)–Zn(1)–O(1)	90.0	O(2)–C(1)–O(1)	121.0(3)
O(2)#1–Zn(1) –O(1)	118.50(9)	O(2)–C(1)–C(2)	119.8(3)
O(2)–Zn(1)–O(1)	61.50(9)	O(1)–C(1)–C(2)	119.3(3)

Symmetry equivalents: #1 -x,-y,-z; #2 -x,y,-z; #3 x,-y,z; #4 -x,-y-1,-z

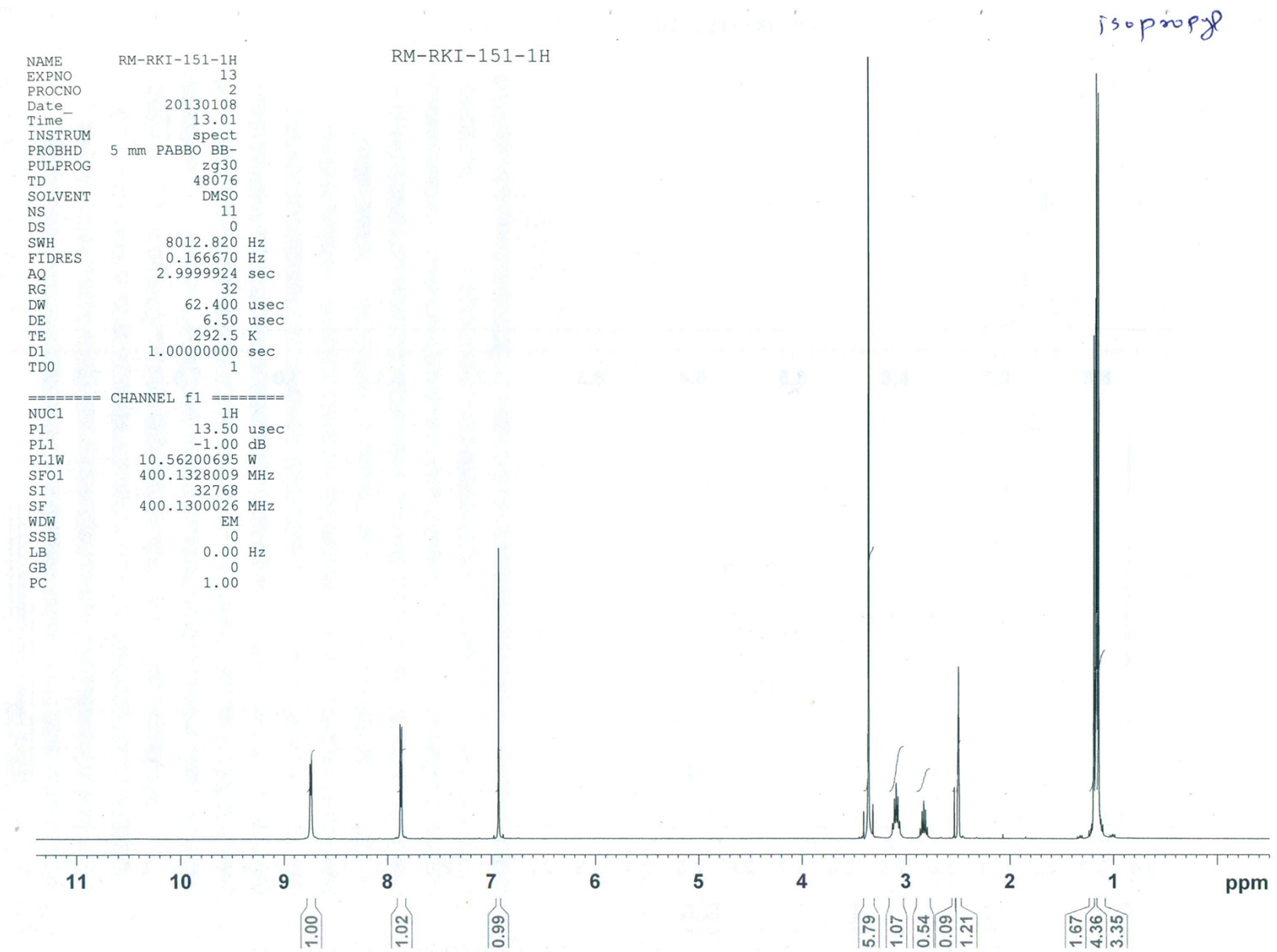

Fig. S9. ^{1}H NMR spectrum of **8** in DMSO-d_6.

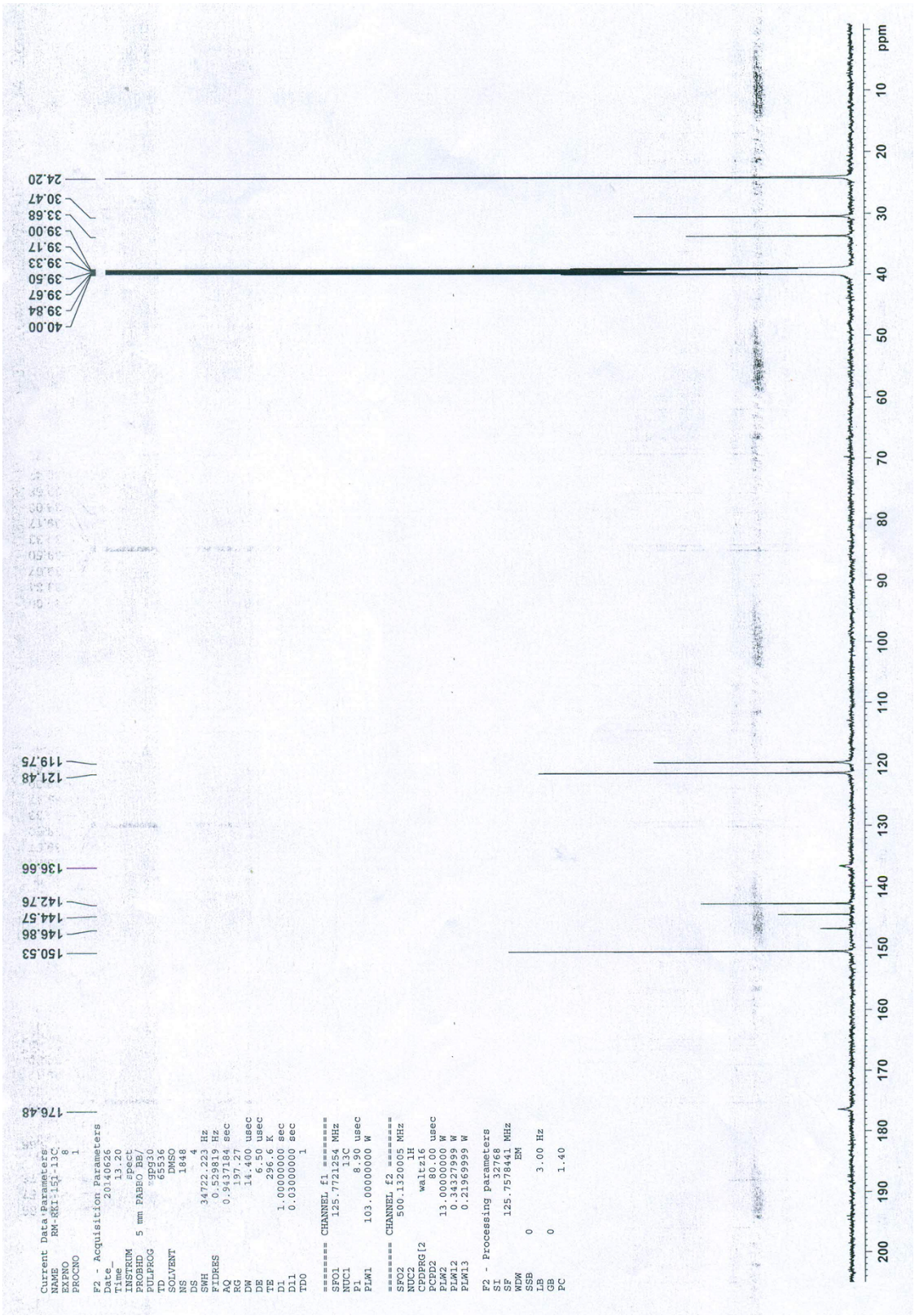

Fig. S10. ^{13}C NMR spectrum of **8** in DMSO-d_6.

Fig. S11. ^{1}H NMR spectrum of **10** in DMSO-d_6.

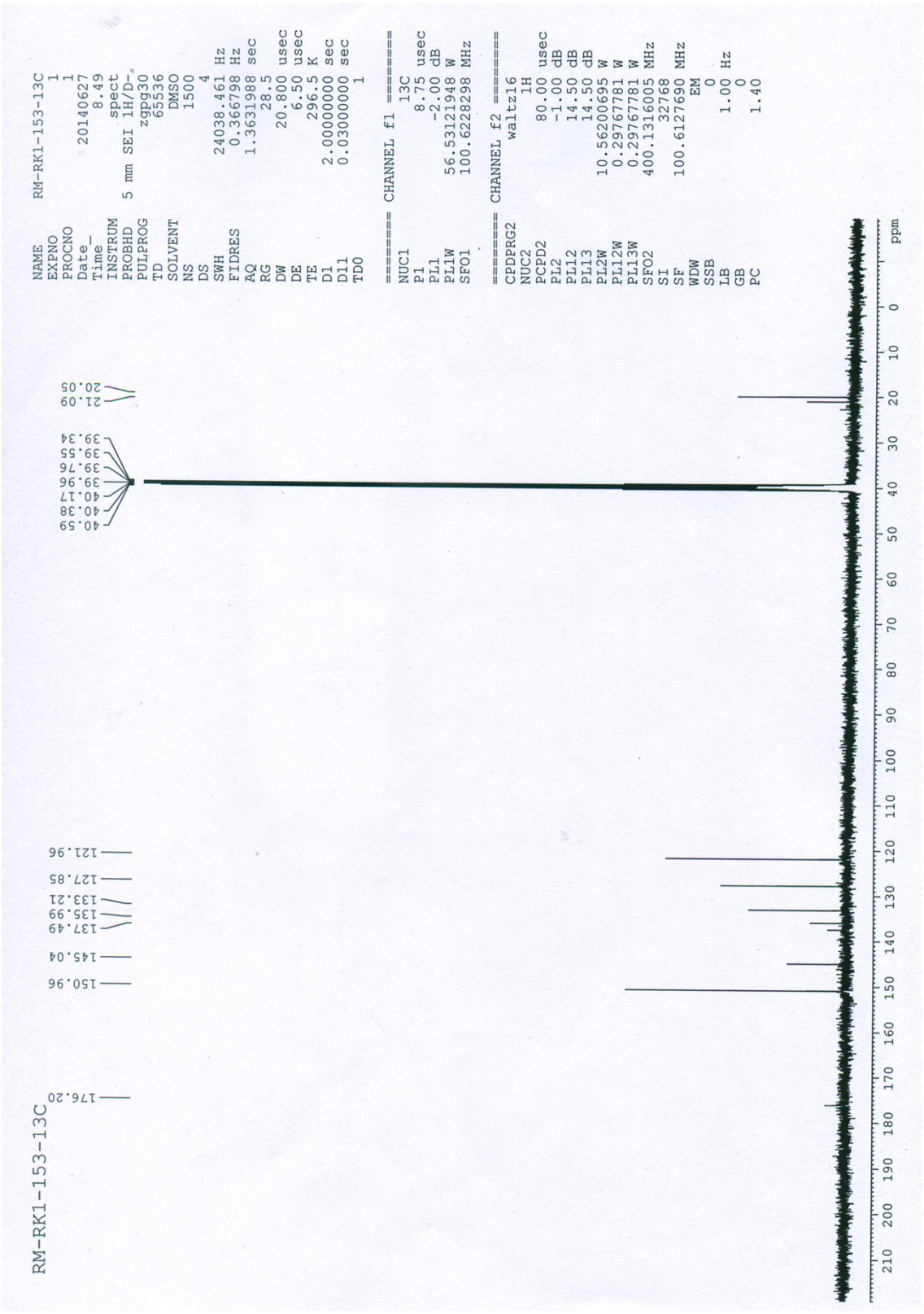

Fig. S12. ^{13}C NMR spectrum of **10** in DMSO-d_6.

Table S10. Comparison of zinc-4,4'-bpy complexes with –O and –N coordination.

Compound	**Geometry around Zn**	**Zn-O (COO^-) (Å)**	**Zn-N (hc) (Å)**	**<N-Zn-N (°)**	**nature of COO^-**	**Type of structure**	**Ref.***
$[Zn(L^2)_2(AL^2)]$ (**8**)	Oh	2.136 2.162	2.130	190	bidentate	1-D linear polymer	this work
$[Zn(L^3)(OAc)(AL^2)]$ (**10**)	Oh	2.450 2.080	2.195 2.190	190	bidentate	Rail-road like polymer	this work
Zn(4,4'-bpy)(4,4'-biphenyl dicarboxylate	T_d	1.91(1) 2.01(1)	2.075(9) 2.111(9)	108.4(7)	monodentate	3-D polymer	20a
$[Zn(H_2O)4$ (4,4'-bpy)] (succinate)$\cdot 4H_2O$	distorted Oh	2.061 Å 2.185 Å	2.132 Å	–	–	2-D layer	20b
$[Zn_2(4,4'\text{-bpy})(btc)(H_2O)]_n\cdot 2nH_2O$[a]	T_d	1.935(2), 1.996(2)	2.0552	–	monodentate	3-D network	20c
$[Zn_4O(ip)_3(4,4'\text{-bpy})]$[b]	T_d	1.970(2), 1.989(2), 1.969(3)	2.076(3)	–	bisbidentate and bismonodentate	2-D grid	20d
$[Zn_4(OH)_2(fa)_3(4,4'\text{-bpy})_2]$[c]	distorted O_h, T_d	2.367(4), 2.089(4), 2.054(4)	2.192(4)	–	chelate monodentate and bisbidentate	3-D framework	20e
Zn(succinate)(4,4'-bpy)	distorted O_h	2.046(5), 2.295(5)	2.097(6)	–	bidentate chelating	layered structure	20f

[a]btc: 1,2,4,5-benzenetetracarboxylic anhydride; [b]ip; isophthalate; [c]fa: fumarate.

* References are included in main text.

Table S11. Selected structural parameters observed in [Mn(L^3)(OAc)(AL^2)] (**9**).

Bond lengths (Å)			
Mn(1)-O(2)	2.095(3)	N(1)-Mn(1)#3	2.303(4)
Mn(1)-O(1)	2.102(3)	O(1)-C(15)#1	1.251(5)
Mn(1)-O(3)	2.231(3)	C(5)-N(2)	1.334(5)
Mn(1)-N(2)	2.276(4)	C(6)-N(2)	1.340(5)
Mn(1)-O(4)	2.298(3)	C(8)-N(1)	1.333(5)
Mn(1)-N(1)#2	2.303(4)	C(9)-N(1)	1.331(5)
Bond angles (°)			
O(2)-Mn(1)-O(1)	123.34(12)	O(1)-Mn(1)-O(4)	148.69(11)
O(2)-Mn(1)-O(3)	145.47(12)	O(3)-Mn(1)-O(4)	57.92(10)
O(1)-Mn(1)-O(3)	90.85(11)	N(2)-Mn(1)-O(4)	92.81(12)
O(2)-Mn(1)-N(2)	87.24(12)	O(2)-Mn(1)-N(1)#2	93.30(13)
O(1)-Mn(1)-N(2)	88.58(12)	O(1)-Mn(1)-N(1)#2	87.66(13)
O(3)-Mn(1)-N(2)	89.16(12)	O(3)-Mn(1)-N(1)#2	92.73(13)
O(2)-Mn(1)-O(4)	87.96(11)	N(2)-Mn(1)-N(1)#2	175.82(12)

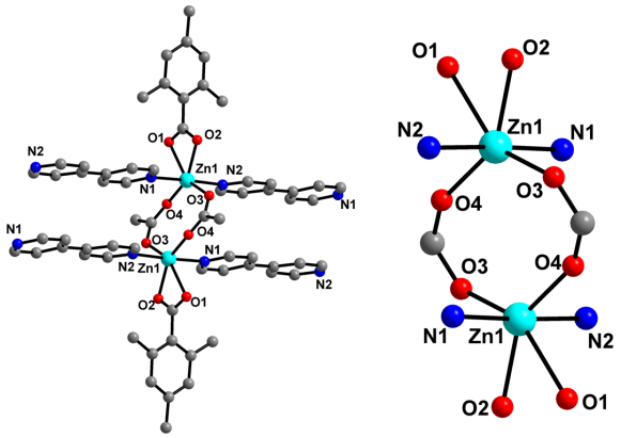

Fig. S13. Molecular structure of zinc polymer **10** and octahedral coordination view of zinc atom.

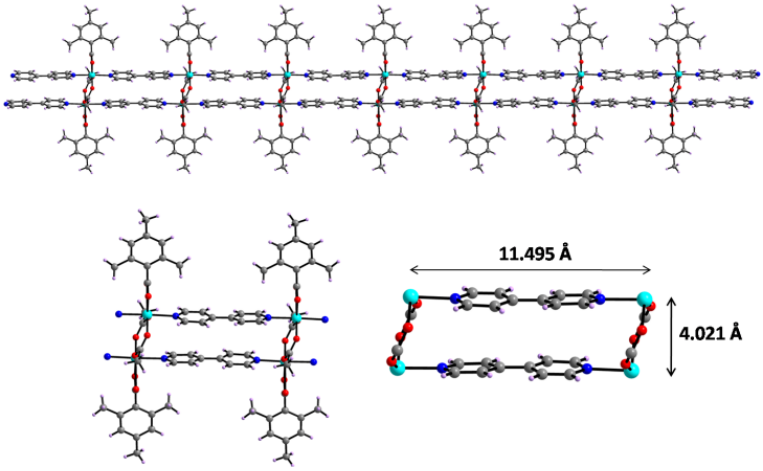

Fig. S14. Rail-road like polymeric view of zinc complex **10** (top) and view of rectangle units are repeated in the polymer with rectangle size (bottom).

Table S12. Selected structural parameters observed in [Zn(L^3)(OAc)(AL^2)] (**9**).

Bond lengths (Å)			
Zn(1)-O(4)	2.025(2)	Zn(1)-C(11)	2.596(3)
Zn(1)-O(3)	2.0295(19)	O(1)-C(11)	1.238(3)
Zn(1)-O(2)	2.0805(19)	O(2)-C(11)	1.253(3)
Zn(1)-N(2)	2.190(2)	O(3)-C(21)	1.243(3)
Zn(1)-N(1)	2.195(2)	O(4)-C(21)#1	1.237(3)
Zn(1)-O(1)	2.450(2)	N(1)-C(5)	1.327(3)
Bond angles (°)			
O(4)-Zn(1)-O(3)	122.48(10)	O(3)-Zn(1)-N(1)	90.67(8)
O(4)-Zn(1)-O(2)	142.13(9)	O(2)-Zn(1)-N(1)	91.39(8)
O(3)-Zn(1)-O(2)	95.18(8)	N(2)-Zn(1)-N(1)	177.70(8)
O(4)-Zn(1)-N(2)	86.73(8)	O(4)-Zn(1)-O(1)	85.73(9)
O(3)-Zn(1)-N(2)	88.46(8)	O(3)-Zn(1)-O(1)	151.79(8)
O(2)-Zn(1)-N(2)	90.81(8)	O(2)-Zn(1)-O(1)	56.65(7)
O(4)-Zn(1)-N(1)	91.94(8)	N(2)-Zn(1)-O(1)	93.16(8)

Fig. S15. ^{1}H NMR spectrum of **11** in DMSO-d_6.

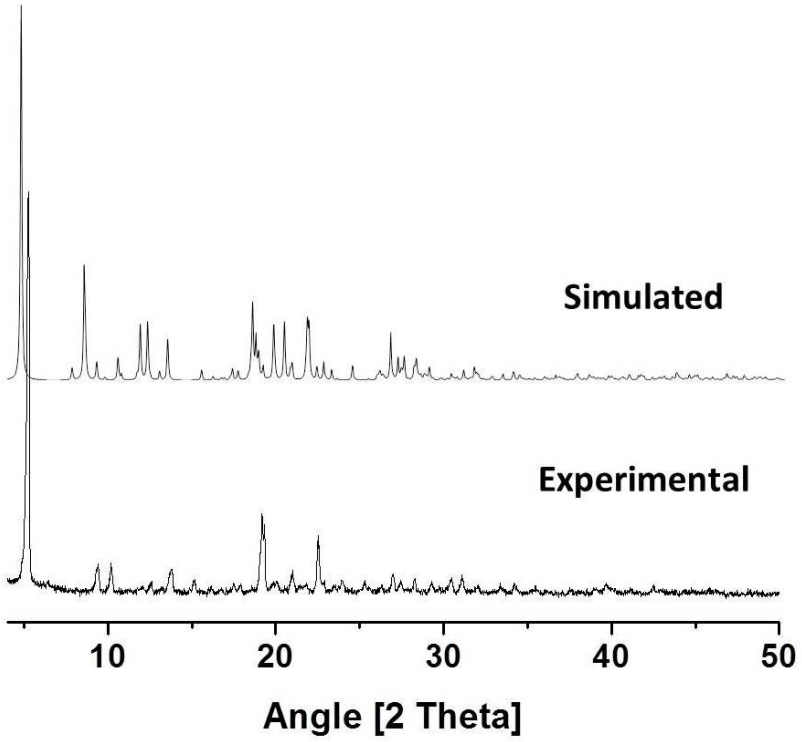

Fig. S16. PXRD pattern of **2**.

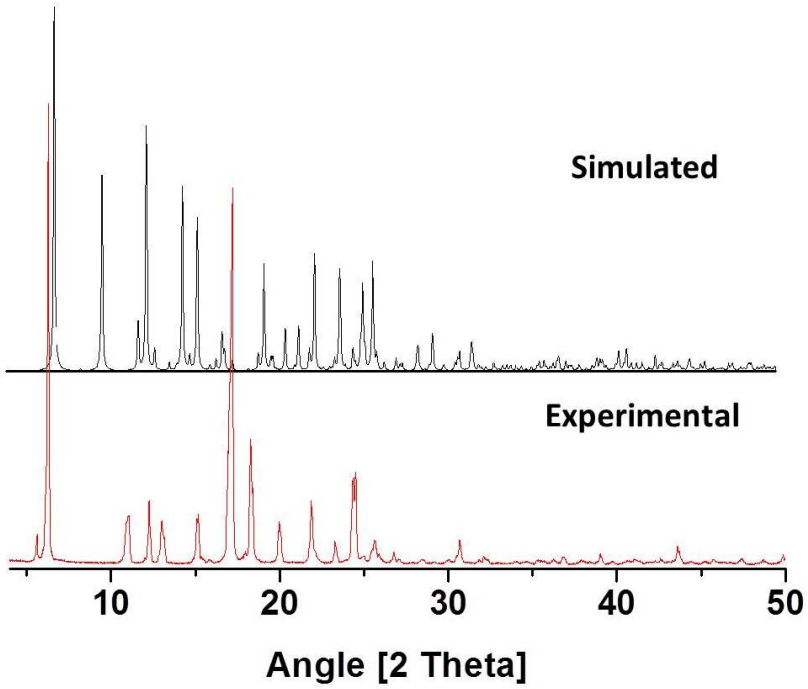

Fig. S17. PXRD pattern of **8**.

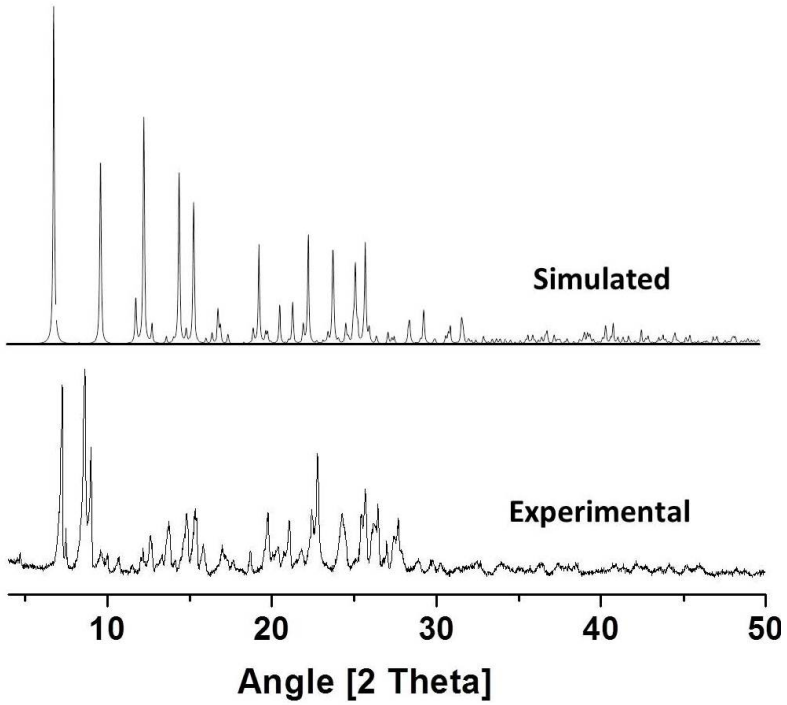

Fig. S18. PXRD pattern of **10**.

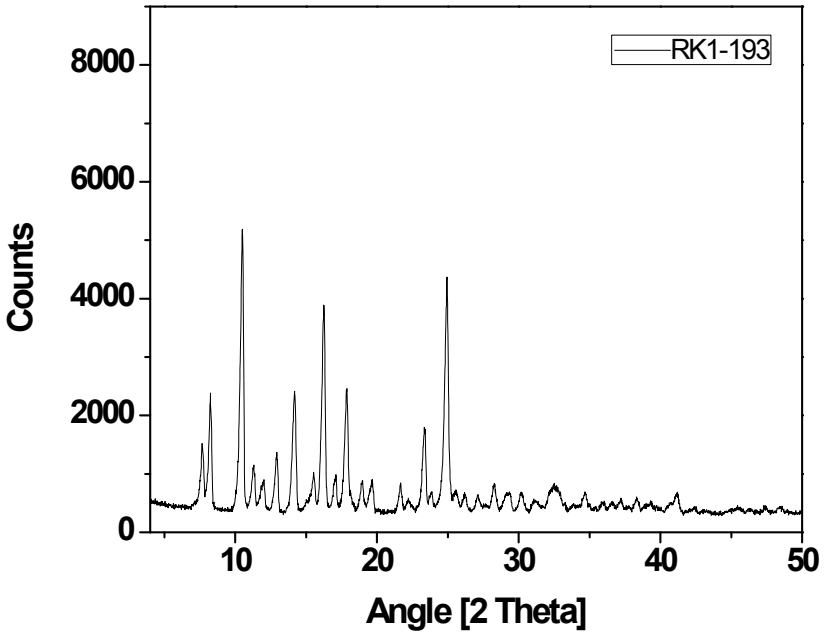

Fig. S19. PXRD pattern of **11**.