Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information for:

H–bond Supported Coordination Polymers of Transition Metal Sulfites with Different Dimensionalities

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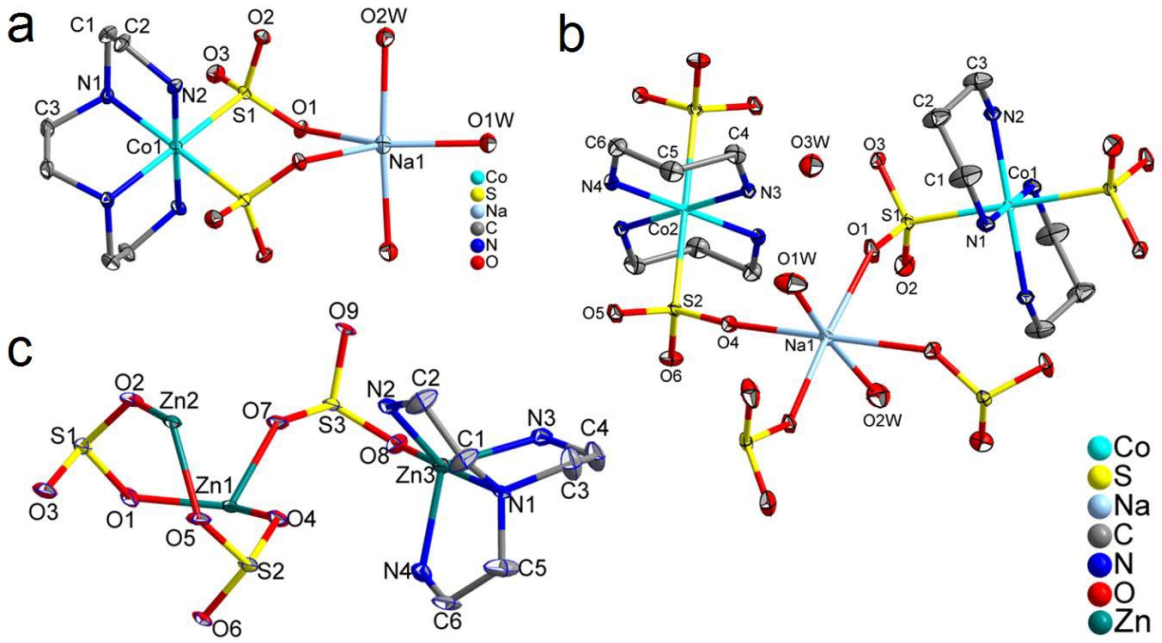

Fig. S1 (a) Molecular structure of $[(C_6N_4H_{18})NaCo(SO_3)_2(H_2O)_3]$, **1**, at 35% ellipsoid probability; (b) Molecular structure of $[(C_3N_2H_{10})_2NaCo(SO_3)_2(H_2O)_2].H_2O$, **2**, at 30 % ellipsoid probability; (c) Asymmetric unit of $[(C_6N_4H_{18})Zn_3(SO_3)_3]$, **3**, with 20 % ellipsoid probability (unique atoms are labelled).

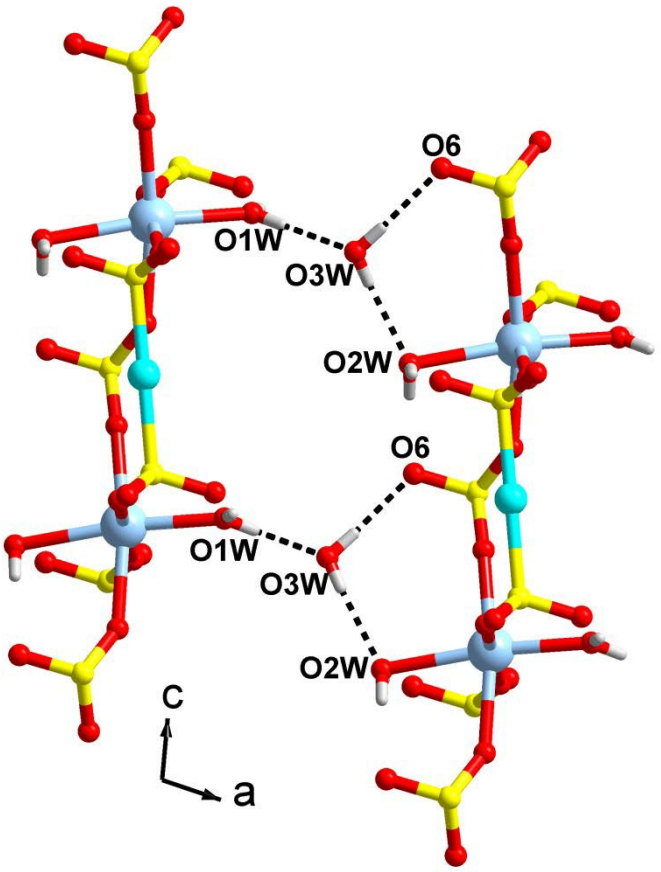

Fig. S2. Interconnection of different layers *via* H-bonding through water molecules in case of $[(C_3N_2H_{10})_2NaCo(SO_3)_2(H_2O)_2].H_2O$, **2**.

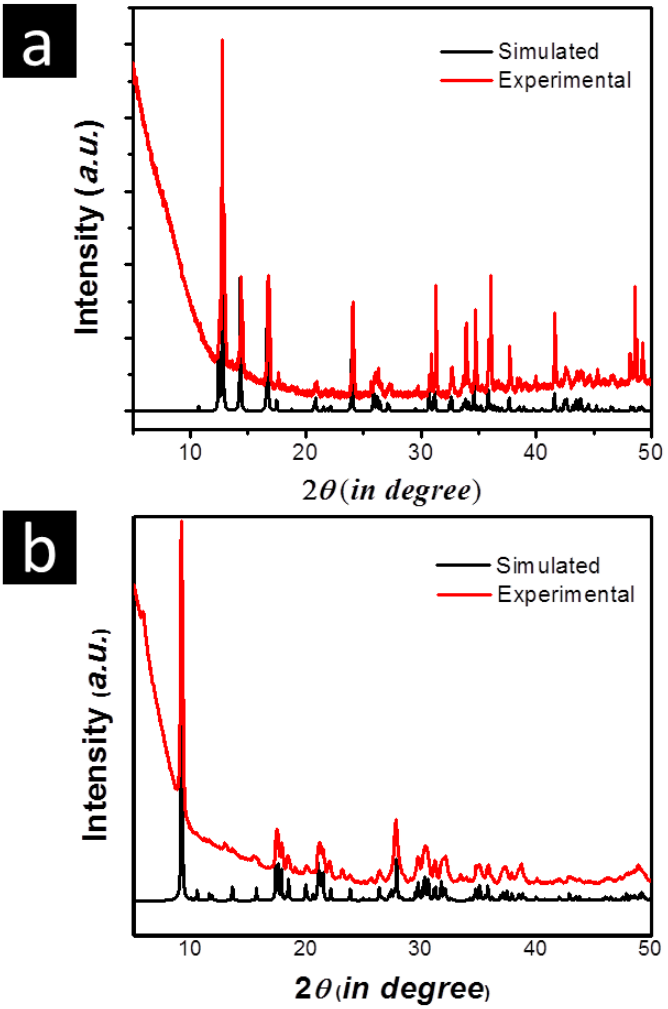

Fig. S3. PXRD pattern for (a) $[(C_6N_4H_{18})NaCo(SO_3)_2(H_2O)_3]$, **(1)** and (b) $[(C_6N_4H_{18})Zn_3(SO_3)_3]$, **(3).**

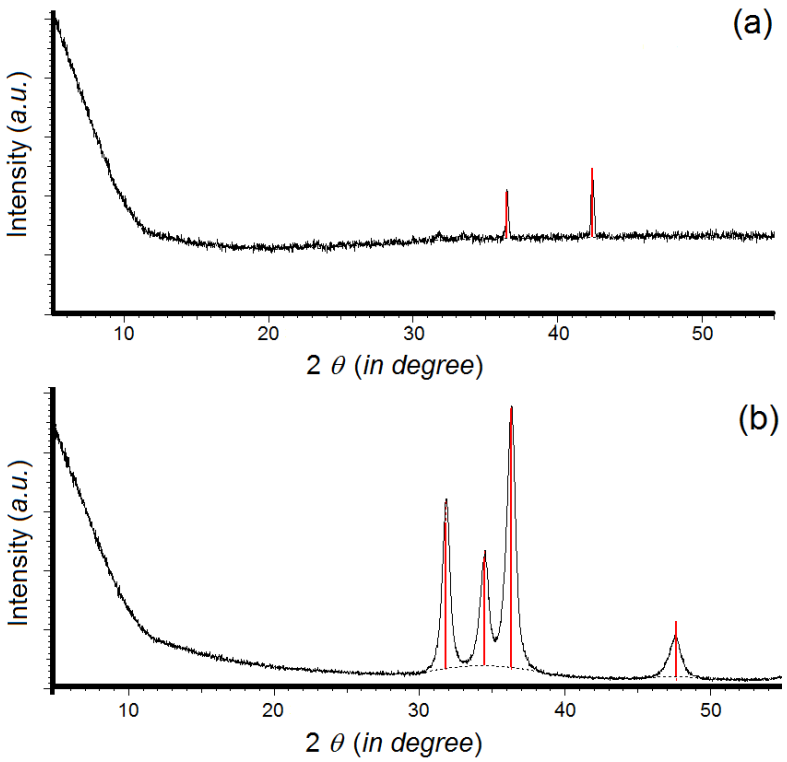

Fig. S4. Post calcination PXRD analysis of (a) $[(C_6N_4H_{18})NaCo(SO_3)_2(H_2O)_3]$, **1**, & $[(C_3N_2H_{10})_2NaCo(SO_3)_2(H_2O)_2].H_2O$, **2** and (b) $[(C_6N_4H_{18})Zn_3(SO_3)_3]$, **3** showing formation of CoO (PDF-00-043-1004) and ZnO (PDF-01-075-0576) respectively.

Table S1. Hydrogen bonding table for **1-3**.[#]

D—H···A	Symmetry of A	D—H	H···A	D—A	∠D—H···A
$[(C_6N_4H_{18})NaCo(SO_3)_2(H_2O)_3]$, 1					
N1—H1···O3		0.88(4)	2.37(4)	2.898(3)	119(3)
N1—H1···O2w	-½+x, ½+y,z	0.88(4)	2.23(4)	2.964(4)	141(4)
N2—H2A···O3	½+x, ½-y, ½+z	0.86(4)	2.26(4)	2.995(4)	144(4)
N2—H2B···O2		0.88(3)	2.13(4)	2.838(4)	138(4)
O1w—H1w1···O3	½-x, -½+y, ½-z	0.83(4)	2.00(4)	2.810(3)	166(4)
O2w—H1w2···O1	1-x, -y, -z	0.82(2)	1.96(2)	2.762(3)	167(5)
O2w—H2w2···O2	1-x, y, ½-z	0.86(3)	1.98(3)	2.770(3)	152(4)
$[(C_3N_2H_{10})_2NaCo(SO_3)_2(H_2O)_2].H_2O$, 2					
N1—H1B···O1	1-x, -y, -z	0.83(3)	2.29(3)	2.855(2)	125(2)
N1—H1B···O5	1-x, -y, -z	0.83(3)	2.22(3)	2.946(2)	146(3)
N2—H2A···O3	1-x, -y, -z	0.85(3)	2.22(3)	2.866(2)	133(2)
N2—H2A···O4	x, ½-y, -½+z	0.85(3)	2.50(3)	3.085(2)	127(2)
N3—H3A···O1		0.84(2)	2.41(2)	2.934(2)	121(2)
N3—H3A···O4		0.84(2)	2.16(3)	2.870(2)	142(2)
N3—H3B···O3		0.84(3)	2.19(3)	3.005(2)	163(2)
N4—H4B···O5	x, ½-y, ½+z	0.86(3)	2.09(3)	2.821(2)	142(2)
O1w—H1w1···O3w	1+x, y, z	0.787(19)	1.979(19)	2.763(3)	175(2)
O1w—H2w1···O2	1-x, ½+y, ½-z	0.85(2)	2.15(2)	2.931(3)	152(3)
O2w—H1w2···O6	x, ½-y, -½+z	0.84(2)	2.17(3)	2.986(3)	164(2)
O2w—H2w2···O2		0.84(2)	2.34(2)	3.136(3)	159(3)
O3w—H1w3···O2w		0.78(3)	2.09(3)	2.846(3)	164(4)
O3w—H2w3···O6		0.81(2)	2.00(2)	2.814(2)	174(3)
C3—H3B···O2		0.97	2.55	3.188(3)	123
C4—H4A···O6	1-x, -y, 1-z	0.97	2.53	3.182(2)	125
$[(C_6N_4H_{18})Zn_3(SO_3)_3]$, 3					
N2—H2A···O2	-x, -y, -z	0.85(11)	2.54(11)	3.008(11)	115(11)
N2—H2A···O7	-x, -y, -z	0.85(11)	2.33(14)	3.015(14)	138(11)
N2—H2B···O4		0.85	2.27	3.031(10)	150
N2—H2B···O9	-x, -y, -z	0.85	2.57	3.079(14)	120
N3—H3A···O6	1-x, -y, -z	0.86(8)	2.40(9)	3.057(14)	134(8)
N3—H3B···O5	1+x, y, -1+z	0.81(10)	2.50(11)	3.089(13)	131(11)
N3—H3B···O2	-x, -y, -z	0.81(10)	2.57(14)	3.158(16)	131(11)
N4—H4A···O4		0.88	2.38	3.125(14)	143
N4—H4B···O3	-x, -y, 1-z	0.86(10)	2.35(10)	3.049(13)	139(7)
C4—H4D···O5	1+x, y, -1+z	0.97	2.48	3.188(15)	130

[#] Where 'D' is donor and 'A' is acceptor, the bond lengths are in (Å) and angles are in (°).

Table S2. Complete list of bond lengths [Å] and bond angles [°] for **1-3**[#]

$[(C_6N_4H_{18})NaCo(SO_3)_2(H_2O)_3]$, 1					
Co1─N1	2.020(3)	Na1─O2w	2.339(3)	C1─C2	1.508(5)
Co1─N2	1.971(3)	S1─O1	1.488(2)	C2─N2	1.485(4)
Co1─S1	2.216(8)	S1─O2	1.485(2)	C3─N1	1.487(4)
Na1─O1	2.349(3)	S1─O3	1.488(2)	C3─C3[a]	1.503(7)
Na1─O1w	2.281(4)	C1─N1	1.497(4)		
N1─Co1─N1[a]	84.97(16)	O1─Na1─O1w	140.01(6)	O1─S1─O3	108.61(13)
N1─Co1─N2	85.14(11)	O1─Na1─O2w	95.46(9)	O2─S1─O3	109.90(15)
N1─Co1─N2[a]	95.71(11)	O1─Na1─O2w[a]	87.77(9)	S1─O1─Na1	124.46(13)
N1─Co1─S1	90.58(8)	O1w─Na1─O2w	87.90(8)	N1─C1─C2	109.5(3)
N1─Co1─S1[a]	171.03(8)	O1w─Na1─O2w[a]	87.90(8)	N2─C2─C1	108.1(3)
N2─Co1─N2[a]	178.86(15)	O2w─Na1─O2w[a]	175.80(15)	C1─N1─Co1	107.76(19)
N2─Co1─S1	91.66(9)	O1─S1─Co1	111.93(10)	C3─N1─Co1	110.4(2)
N2─Co1─S1[a]	87.57(8)	O2─S1─Co1	109.95(10)	C3─N1─C1	113.1(3)
S1─Co1─S1[a]	94.85(4)	O3─S1─Co1	106.86(10)	C2─N2─Co1	112.1(2)
O1─Na1─O1[a]	79.99(12)	O1─S1─O2	109.54(13)	N1─C3─C3[a]	110.8(2)
$[(C_3N_2H_{10})_2NaCo(SO_3)_2(H_2O)_2].H_2O$, 2					
Co1─N1	1.988(2)	Na1─O5[c]	2.401(1)	C1─C2	1.479(3)
Co1─N2	1.978(2)	Na1─O1w	2.337(2)	C2─C3	1.475(3)
Co1─S1	2.259(4)	Na1─O2w	2.563(2)	C4─C5	1.508(3)
Co2─N3	1.971(1)	S1─O1	1.485(2)	C5─C6	1.510(3)
Co2─N4	1.987(2)	S1─O2	1.479(2)	C1─N1	1.472(3)
Co2─S2	2.273(4)	S1─O3	1.492(1)	C3─N2	1.476(3)
Na1─O1	2.319(2)	S2─O4	1.488(1)	C4─N3	1.480(2)
Na1─O3[b]	2.379(1)	S2─O5	1.491(1)	C6─N4	1.485(2)
Na1─O4	2.389(1)	S2─O6	1.487(1)		
N1─Co1─N1[d]	180.0	O1─Na1─O5[c]	82.71(5)	O6─S2─O4	108.87(8)
N1─Co1─N2	94.34(6)	O1─Na1─O1w	97.91(7)	O4─S2─O5	109.17(8)
N1─Co1─N2[d]	85.66(7)	O1─Na1─O2w	81.03(7)	O6─S2─Co2	113.31(6)
N1─Co1─S1	89.41(5)	O3[b]─Na1─O4	93.92(5)	O4─S2─Co2	109.38(5)
N1─Co1─S1[d]	90.59(5)	O3[b]─Na1─O5[c]	91.84(5)	O5─S2─Co2	108.65(6)
N2─Co1─N2[d]	180.0	O3[b]─Na1─O2w	100.74(7)	N1─C1─C2	115.75(19)
N2─Co1─S1	89.52(5)	O4─Na1─O5[c]	170.32(6)	C3─C2─C1	115.2(2)
N2─Co1─S1[d]	90.48(5)	O4─Na1─O2w	92.27(6)	C2─C3─N2	114.01(19)
N3─Co2─N3[e]	180.0	O5[c]─Na1─O2w	79.01(6)	N3─C4─C5	111.98(15)
N3─Co2─N4	94.76(6)	O1w─Na1─O3[b]	79.68(6)	C4─C5─C6	112.01(17)
N3─Co2─N4[e]	85.24(7)	O1w─Na1─O4	94.03(7)	N4─C6─C5	112.14(17)
N3─Co2─S2	90.25(5)	O1w─Na1─O5[c]	94.64(7)	C1─N1─Co1	125.30(13)
N3─Co2─S2[e]	89.75(5)	O1w─Na1─O2w	173.64(8)	C3─N2─Co1	123.71(13)
N4─Co2─N4[e]	180.0	O1─S1─O2	108.35(10)	C4─N3─Co2	124.39(12)
N4─Co2-S2	90.04(5)	O1─S1─O3	108.86(9)	C6─N4─Co2	123.73(12)
N4─Co2-S2[e]	89.96(5)	O2─S1─O3	108.80(9)	S1─O1─Na1	152.26(12)
S1─Co1─S1[d]	180.0	O2─S1─Co1	111.61(7)	S1─O3─Na1[f]	144.26(9)
S2─Co2─S2[e]	180.0	O1─S1─Co1	109.47(6)	S2─O4─Na1	170.70(9)
O1─Na1─O3[b]	173.87(6)	O3─S1─Co1	109.69(5)	S2─O5─Na1[g]	143.27(8)
O1─Na1─O4	91.87(5)				
$[(C_6N_4H_{18})Zn_3(SO_3)_3]$, 3					

Zn1─O1	1.925(7)	Zn3─N3	2.058(10)	O9─S3	1.504(7)
Zn1─O4	1.977(8)	Zn3─N4	2.075(9)	C1─N1	1.428(14)
Zn1─O6^{h}	1.953(7)	O1─S1	1.508(7)	C1─C2	1.431(16)
Zn1─O7	1.939(7)	O2─S1	1.538(7)	C2─N2	1.428(16)
Zn2─O2	1.934(8)	O3─S1	1.513(8)	C3─C4	1.421(17)
Zn2─O3^{i}	1.962(7)	O4─S2	1.528(7)	C3─N1	1.453(14)
Zn2─O5	1.954(7)	O5─S2	1.501(7)	C4─N3	1.453(15)
Zn2─O9^{j}	1.936(7)	O6─S2	1.526(7)	C5─C6	1.404(16)
Zn3─O8	2.037(8)	O7─S3	1.506(8)	C5─N1	1.462(13)
Zn3─N1	2.262(9)	O8─S3	1.505(7)	C6─N4	1.445(14)
Zn3─N2	2.024(9)				
O1─Zn1─O4	117.5(3)	N2─Zn3─N3	119.7(3)	C2─N2─Zn3	113.5(8)
O1─Zn1─O6^{h}	110.5(3)	N2─Zn3─N4	115.3(3)	C4─N3─Zn3	113.5(8)
O1─Zn1─O7	113.1(3)	N3─Zn3─N4	116.8(3)	C6─N4─Zn3	112.2(7)
O4─Zn1─O6^{h}	104.7(3)	O1─S1─O3	103.7(4)	S2─O4─Zn1	122.9(4)
O4─Zn1─O7	98.6(3)	O1─S1─O2	105.1(4)	S2─O5─Zn2	129.3(4)
O7─Zn1─O6^{h}	111.7(3)	O2─S1─O3	104.5(5)	S2─O6─Zn1^{h}	128.7(4)
O2─Zn2─O3^{i}	105.7(4)	O4─S2─O5	105.1(4)	S3─O7─Zn1	136.3(5)
O2─Zn2─O5	117.7(3)	O6─S2─O4	105.6(4)	S3─O8─Zn3	133.2(5)
O2─Zn2─O9^{j}	103.2(4)	O5─S2─O6	104.8(4)	S3─O9─Zn2^{j}	135.6(5)
O3^{i}─Zn2─O5	108.3(3)	O8─S3─O9	106.4(5)	S1─O1─Zn1	131.3(4)
O3^{i}─Zn2─O9^{j}	111.8(3)	O7─S3─O9	101.1(5)	S1─O2─Zn2	126.8(5)
O5─Zn2─O9^{j}	110.0(3)	O7─S3─O8	106.2(5)	S1─O3─Zn2^{i}	129.4(4)
N1─Zn3─O8	174.7(3)	C1─N1─C3	113.7(10)	N1─C1─C2	114.6(11)
N2─Zn3─O8	104.4(4)	C1─N1─C5	112.3(10)	N2─C2─C1	115.8(11)
N3─Zn3─O8	94.8(3)	C3─N1─C5	111.6(11)	C4─C3─N1	116.7(11)
N4─Zn3─O8	99.6(3)	C1─N1─Zn3	106.9(7)	C3─C4─N3	114.7(11)
N1─Zn3─N2	80.1(3)	C3─N1─Zn3	106.0(7)	C6─C5─N1	116.3(11)
N1─Zn3─N3	80.5(4)	C5─N1─Zn3	105.7(7)	C5─C6─N4	116.6(10)
N1─Zn3─N4	80.7(3)				

[#]Symmetry transformations used to generate equivalent atoms: (a) -x, y, -z+3/2; (b) -x+1, y-1/2, -z-1/2; (c) x, -y+1/2, z-1/2; (d) -x+1, -y+1, -z-1; (e) -x+1, -y+1, -z; (f) -x+1, y+1/2, -z-1/2; (g) x, -y+1/2, z+1/2; (h) -x, -y, -z+1; (i) -x-1, -y, -z+1; (j) -x, -y, -z

Table S3. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters (Å$\times 10^3$) for **1-3** U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
$[(C_6N_4H_{18})NaCo(SO_3)_2(H_2O)_3]$, 1				
Co1	0	2274(1)	7500	14(1)
S1	1609(1)	3330(1)	7664(1)	17(1)
Na1	0	5444(1)	7500	29(1)
C1	1725(4)	1256(2)	6117(3)	27(1)
C2	548(4)	1491(2)	5156(3)	28(1)
C3	735(4)	306(2)	7691(4)	31(1)
N1	1313(3)	1226(2)	7400(2)	20(1)
N2	-164(3)	2288(2)	5649(2)	20(1)
O1	1290(2)	4177(2)	8377(2)	23(1)
O2	1871(2)	3614(2)	6392(2)	25(1)
O3	2799(2)	2871(2)	8363(2)	26(1)
O1w	0	7049(3)	7500	44(1)
O2w	-1353(3)	5504(2)	9079(2)	32(1)
$[(C_3N_2H_{10})_2NaCo(SO_3)_2(H_2O)_2].H_2O$, 2				
Co1	5000	5000	-5000	15(1)
Co2	5000	5000	0	14(1)
Na1	4834(1)	2431(1)	-2503(1)	25(1)
S1	4543(1)	4937(1)	-3474(1)	22(1)
S2	4082(1)	3455(1)	-78(1)	17(1)
C1	1908(3)	6121(2)	-5702(2)	50(1)
C2	1308(3)	5246(2)	-6281(2)	45(1)
C3	1623(3)	4321(2)	-5741(2)	45(1)
C4	7959(2)	4474(2)	-680(2)	29(1)
C5	8422(2)	3880(2)	250(2)	32(1)
C6	8309(2)	4454(2)	1151(2)	31(1)
N1	3610(2)	6151(1)	-5296(1)	23(1)
N2	3294(2)	4055(1)	-5461(1)	22(1)
N3	6261(2)	4675(1)	-951(1)	20(1)
N4	6663(2)	4657(1)	1181(1)	22(1)
O1	5155(2)	4010(1)	-2993(1)	42(1)
O2	2852(2)	4993(1)	-3508(1)	45(1)
O3	5354(2)	5758(1)	-2869(1)	25(1)
O4	4399(2)	2965(1)	-961(1)	30(1)
O5	4913(2)	2926(1)	825(1)	26(1)
O6	2379(2)	3397(1)	-122(1)	31(1)
O1w	7469(2)	2068(2)	-1853(2)	56(1)
O2w	2003(2)	2793(2)	-3405(2)	48(1)
O3w	10289(2)	2917(2)	-1914(2)	49(1)
$[(C_6N_4H_{18})Zn_3(SO_3)_3]$, 3				
Zn1	-17(1)	-905(1)	3618(1)	35(1)
Zn2	-3378(1)	996(1)	3050(1)	35(1)
Zn3	3257(1)	1563(1)	-536(1)	36(1)
S1	-3313(3)	-2027(3)	5104(3)	37(1)
S2	-1229(3)	2021(3)	3932(3)	36(1)
S3	2423(3)	-1722(3)	557(3)	34(1)

C1	1797(14)	4350(14)	-1233(18)	65(4)
C2	1056(16)	3346(15)	-1368(18)	72(4)
C3	4502(15)	4347(14)	-2848(15)	71(4)
C4	5721(14)	3387(14)	-3235(14)	61(4)
C5	3480(20)	4331(14)	-181(15)	76(5)
C6	3023(17)	3363(13)	1299(13)	60(4)
N1	3242(9)	3921(9)	-1294(9)	32(2)
N2	1273(10)	1920(10)	-651(9)	38(2)
N3	5274(10)	1930(11)	-2552(12)	40(2)
N4	3222(10)	1906(10)	1364(9)	42(2)
O1	-1846(8)	-1943(9)	5138(8)	45(2)
O2	-3118(9)	-1006(8)	3535(8)	46(2)
O3	-4449(8)	-1324(10)	6299(8)	53(2)
O4	-195(8)	1142(8)	2864(8)	40(2)
O5	-2753(8)	1977(8)	4017(8)	42(2)
O6	-1427(8)	1185(8)	5552(7)	42(2)
O7	882(8)	-1304(10)	1641(8)	54(2)
O8	3481(9)	-552(8)	33(9)	47(2)
O9	2189(9)	-1631(10)	-812(8)	59(3)

Table S4. Anisotropic displacement parameters ($Å^2 \times 10^3$) for **1-3**. The anisotropic displacement factor exponent takes the form: $-2\ pi^2\ [h^2\ a^{*2}\ U_{11} + ... + 2\ h\ k\ a^*\ b^*\ U_{12}]$

	U11	U22	U33	U23	U13	U12
$[(C_6N_4H_{18})NaCo(SO_3)_2(H_2O)_3]$, 1						
Co1	14(1)	13(1)	15(1)	0	1(1)	0
S1	15(1)	17(1)	18(1)	-1(1)	2(1)	-2(1)
Na1	32(1)	22(1)	35(1)	0	7(1)	0
C1	25(2)	27(2)	28(2)	-3(1)	6(2)	7(1)
C2	36(2)	27(2)	22(2)	-6(1)	7(2)	8(2)
C3	27(2)	16(1)	51(2)	3(2)	7(2)	3(1)
N1	19(1)	17(1)	23(1)	0(1)	1(1)	2(1)
N2	17(1)	22(1)	19(1)	-2(1)	0(1)	3(1)
O1	27(1)	18(1)	24(1)	-5(1)	3(1)	0(1)
O2	30(1)	25(1)	22(1)	1(1)	9(1)	-6(1)
O3	16(1)	28(1)	33(1)	-1(1)	-2(1)	2(1)
O1w	38(3)	24(2)	77(3)	0	27(2)	0
O2w	42(2)	28(1)	24(1)	1(1)	4(1)	-2(1)
$[(C_3N_2H_{10})_2NaCo(SO_3)_2(H_2O)_2].H_2O$, 2						
Co1	21(1)	11(1)	14(1)	0(1)	5(1)	-1(1)
Co2	17(1)	12(1)	12(1)	0(1)	4(1)	-1(1)
Na1	37(1)	17(1)	22(1)	0(1)	10(1)	1(1)
S1	35(1)	18(1)	14(1)	-2(1)	10(1)	-6(1)
S2	24(1)	12(1)	18(1)	-1(1)	8(1)	-3(1)
C1	32(1)	30(1)	77(2)	-7(1)	-8(1)	7(1)
C2	32(1)	37(1)	56(2)	-1(1)	-10(1)	0(1)
N4	24(1)	22(1)	18(1)	3(1)	3(1)	-2(1)
O1	92(1)	16(1)	22(1)	3(1)	19(1)	-3(1)
O2	33(1)	71(1)	35(1)	-14(1)	19(1)	-14(1)
O3	40(1)	17(1)	18(1)	-4(1)	8(1)	-2(1)
O4	50(1)	21(1)	23(1)	-9(1)	19(1)	-11(1)
C3	29(1)	34(1)	65(2)	-5(1)	0(1)	-6(1)
C4	26(1)	30(1)	35(1)	-3(1)	16(1)	1(1)
C5	26(1)	28(1)	43(1)	3(1)	9(1)	6(1)
C6	21(1)	37(1)	31(1)	6(1)	0(1)	0(1)
N1	27(1)	16(1)	25(1)	1(1)	6(1)	1(1)
N2	26(1)	17(1)	24(1)	-3(1)	8(1)	-4(1)
N3	25(1)	19(1)	18(1)	-2(1)	9(1)	-3(1)
O5	39(1)	18(1)	22(1)	6(1)	9(1)	1(1)
O6	24(1)	26(1)	43(1)	-2(1)	10(1)	-6(1)
O1w	32(1)	49(1)	87(2)	6(1)	13(1)	-3(1)
O2w	47(1)	56(1)	48(1)	-7(1)	24(1)	-5(1)
O3w	33(1)	71(1)	44(1)	0(1)	9(1)	-8(1)
$[(C_6N_4H_{18})Zn_3(SO_3)_3]$, 3						
C1	46(8)	75(10)	102(11)	-34(8)	-51(8)	6(7)
C2	56(9)	79(11)	115(13)	-37(9)	-62(10)	10(8)
C3	59(9)	60(9)	55(9)	-14(7)	2(7)	-4(7)
C4	38(8)	73(10)	45(8)	-25(7)	5(6)	4(7)
C5	134(15)	64(9)	69(10)	-21(8)	-78(11)	6(9)
C6	98(12)	62(9)	45(8)	-26(6)	-43(8)	-2(8)

N1	26(5)	54(6)	20(4)	-19(4)	-12(4)	6(4)
N2	35(5)	57(6)	28(5)	-23(4)	-12(4)	0(4)
N3	31(5)	60(6)	42(5)	-25(5)	-22(5)	7(5)
N4	36(6)	62(6)	28(5)	-13(4)	-17(4)	2(5)
O1	24(4)	83(6)	24(4)	-9(4)	-11(3)	-3(4)
O2	55(5)	67(5)	26(4)	-13(4)	-24(4)	-6(4)
O3	29(4)	113(7)	32(4)	-37(4)	-17(4)	8(4)
O4	39(4)	59(5)	24(4)	-23(3)	-10(3)	4(4)
O5	30(4)	78(6)	38(4)	-37(4)	-24(4)	13(4)
O6	28(4)	83(6)	17(4)	-20(4)	-9(3)	2(4)
O7	30(4)	110(7)	35(5)	-48(5)	-6(4)	-8(4)
O8	41(5)	59(5)	50(5)	-20(4)	-23(4)	-11(4)
O9	40(5)	126(8)	18(4)	-31(4)	-8(4)	-20(5)
S1	29(2)	60(2)	27(1)	-17(1)	-12(1)	-3(1)
S2	31(2)	59(2)	28(1)	-23(1)	-17(1)	6(1)
S3	31(2)	57(2)	22(1)	-20(1)	-13(1)	0(1)
Zn1	27(1)	67(1)	22(1)	-23(1)	-12(1)	0(1)
Zn2	26(1)	63(1)	23(1)	-22(1)	-12(1)	0(1)
Zn3	32(1)	54(1)	30(1)	-19(1)	-16(1)	0(1)