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Supporting information

Racemic cobalt phosphonates incorporating flexible bis(imidazole) co-ligands

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Table S1. Selected bond lengths (Å) and angles (°) for compound **1**.

Co1-O1A	2.086(4)	Co1-O1W	2.194(4)
Co1-O4	2.088(4)	Co2-O2	2.088(4)
Co1-O3	2.098(4)	Co2-N2	2.123(5)
Co1-N5B	2.101(5)	Co2-O2W	2.157(4)
Co1-N1	2.162(5)		
O1A-Co1-O4	91.74(18)	O3-Co1-O1W	86.85(17)
O1A-Co1-O3	99.00(16)	N5B-Co1-O1W	87.4(2)
O4-Co1-O3	166.11(17)	N1-Co1-O1W	95.84(18)
O1A-Co1-N5B	89.86(19)	O2-Co2-O2C	180.000(1)
O4-Co1-N5B	90.20(19)	O2-Co2-N2	91.72(19)
O3-Co1-N5B	98.56(19)	O2-Co2-N2C	88.28(18)
O1A-Co1-N1	86.71(18)	N2-Co2-N2C	180.000(1)
O4-Co1-N1	88.11(17)	O2-Co2-O2WC	88.12(16)
O3-Co1-N1	83.77(17)	N2-Co2-O2WC	87.6(2)
N5B-Co1-N1	176.1(2)	O2-Co2-O2W	91.88(16)
O1A-Co1-O1W	173.86(17)	N2-Co2-O2W	92.37(19)
O4-Co1-O1W	82.78(18)	O2WC-Co2-O2W	180.00(13)

Symmetry codes: A: -x,-y+1,-z+1; B: -x+1,-y+1,-z+1; C: -x,-y+1,-z+2.

Table S2 Selected bond lengths (Å) and angles (°) for **2**.

Co1-O4	2.091(3)	Co2-N6B	2.124(3)
Co1-O6	2.092(2)	Co2-O2W	2.179(2)
Co1-N3A	2.098(3)	Co2-N2	2.181(3)
Co1-O3	2.104(2)	Co3-O2	2.062(2)
Co1-N1	2.138(3)	Co3-O8C	2.093(2)
Co1-O1W	2.191(2)	Co3-N5	2.132(3)
Co2-O1	2.078(2)	Co3-N4	2.150(3)
Co2-O9	2.078(3)	Co3-O3W	2.168(2)
Co2-O7	2.114(2)	Co3-O4W	2.181(3)
O4-Co1-O6	89.97(10)	O7-Co2-O2W	88.29(9)
O4-Co1-N3A	90.90(11)	N6B-Co2-O2W	86.45(11)
O6-Co1-N3A	91.58(10)	O1-Co2-N2	91.59(10)
O4-Co1-O3	168.99(9)	O9-Co2-N2	89.73(10)
O6-Co1-O3	98.36(9)	O7-Co2-N2	83.19(10)
N3A-Co1-O3	96.03(11)	N6B-Co2-N2	176.92(11)
O4-Co1-N1	88.85(10)	O2W-Co2-N2	93.01(10)
O6-Co1-N1	88.35(10)	O2-Co3-O8C	177.77(10)
N3A-Co1-N1	179.74(13)	O2-Co3-N5	90.71(11)
O3-Co1-N1	84.23(10)	O8C-Co3-N5	90.47(10)
O4-Co1-O1W	83.67(10)	O2-Co3-N4	91.91(11)
O6-Co1-O1W	172.81(9)	O8C-Co3-N4	87.02(11)
N3A-Co1-O1W	85.19(11)	N5-Co3-N4	175.56(12)
O3-Co1-O1W	88.38(9)	O2-Co3-O3W	90.10(9)
N1-Co1-O1W	94.86(10)	O8C-Co3-O3W	91.84(9)
O1-Co2-O9	88.54(10)	N5-Co3-O3W	87.05(11)
O1-Co2-O7	97.22(9)	N4-Co3-O3W	89.37(11)
O9-Co2-O7	170.97(9)	O2-Co3-O4W	91.18(9)
O1-Co2-N6B	89.21(11)	O8C-Co3-O4W	86.83(9)
O9-Co2-N6B	93.27(11)	N5-Co3-O4W	95.28(11)
O7-Co2-N6B	93.76(11)	N4-Co3-O4W	88.25(12)
O1-Co2-O2W	173.21(9)	O3W-Co3-O4W	177.33(10)
O9-Co2-O2W	86.49(10)		

Symmetry codes: A: x+1, y, z-1; B: x-1, y, z; C: x, y, z+1; D: x-1, y, z+1; E: x+1, y, z; F: x, y, z-1.

Table S3 Selected bond lengths (Å) and angles (°) for **3**.

Co1-O1A	2.072(2)	Co1-O1W	2.221(2)
Co1-O4	2.092(2)	Co2-N4	2.109(3)
Co1-N2B	2.109(3)	Co2-O2	2.130(2)
Co1-O3	2.124(2)	Co2-O2W	2.140(2)
Co1-N1	2.153(3)		
O1A-Co1-O4	90.60(9)	N2B-Co1-O1W	89.65(10)
O1A-Co1-N2B	90.62(10)	O3-Co1-O1W	88.25(9)
O4-Co1-N2B	89.61(10)	N1-Co1-O1W	89.11(9)
O1A-Co1-O3	97.46(9)	N4-Co2-N4C	180
O4-Co1-O3	169.93(9)	N4-Co2-O2C	88.57(9)
N2B-Co1-O3	96.30(10)	N4-Co2-O2	91.43(9)
O1A-Co1-N1	90.66(9)	O2C-Co2-O2	180
O4-Co1-N1	90.54(9)	N4-Co2-O2WC	93.35(10)
N2B-Co1-N1	178.72(11)	O2-Co2-O2WC	90.09(8)
O3-Co1-N1	83.37(9)	N4-Co2-O2W	86.65(10)
O1A-Co1-O1W	174.22(9)	O2-Co2-O2W	89.91(8)
O4-Co1-O1W	83.63(9)	O2WC-Co2-O2W	180.000(1)

Symmetry codes: A: -x+2, -y+1, -z+1; B: x+1, y-1, z; C: -x+2, -y+2, -z+1; D: x-1, y+1, z.

Table S4. Selected bond lengths (Å) and angles (°) for **4.**

Co1-O3A	1.954(5)	Co1-N1	2.254(7)
Co1-O1	1.988(4)	Co2-O2	1.933(4)
Co1-O4	2.014(5)	Co2-N4	2.017(5)
Co1-N2	2.081(5)		
O3A-Co1-O1	108.5(2)	O1-Co1-N1	82.4(2)
O3A-Co1-O4	124.7(3)	O4-Co1-N1	78.4(3)
O1-Co1-O4	124.9(3)	N2-Co1-N1	164.4(2)
O3A-Co1-N2	99.0(2)	O2-Co2-O2B	103.0(2)
O1-Co1-N2	91.85(19)	O2-Co2-N4	113.85(18)
O4-Co1-N2	93.2(2)	O2-Co2-N4B	110.85(18)
O3A-Co1-N1	96.7(2)	N4-Co2-N4B	104.7(3)

Symmetry codes: A: -x+2, -y, -z; B: -x+2, y, -z+1/2.

Table S5. Hydrogen bonding parameters for **1**.

D-H...A	d(D-H) (Å)	d(H...A) (Å)	d(D...A)(Å)	<(D-H...A) (°)
C(1)-H(1B)...O(5)#4	0.97	2.65	3.503(8)	146.2
C(2)-H(2)...O(5)#4	0.98	2.44	3.352(8)	154.7
C(23)-H(23)...O(3W)#2	0.93	2.44	3.334(13)	161.8
N(1)-H(1)...O(3)#1	0.98	2.13	3.056(7)	156.7
O(1W)-H(1WA)...O(5)#4	0.85	1.91	2.753(7)	172.1
O(1W)-H(1WB)...O(4W)	0.85	2.08	2.896(8)	161.9
O(2W)-H(2WA)...O(1)	0.85	1.83	2.644(6)	158.9
O(2W)-H(2WB)...O(5)#1	0.85	2.13	2.960(7)	164.4
O(3W)-H(3WA)...O(3)	0.85	2.03	2.870(8)	168
O(3W)-H(3WB)...O(4W)	0.85	2.27	2.982(10)	140.8
O(4W)-H(4WA)...O(4)#4	0.85	2.49	2.989(7)	118.5
O(4W)-H(4WB)...O(2)	0.85	2.13	2.767(7)	131.6
O(4W)-H(4WB)...O(2W)#3	0.85	2.46	3.211(7)	147.5

Symmetry codes: #1: -x, -y+1, -z+1; #2: -x+1, -y+1, -z+1; #3: -x, -y+1, -z+2; #4: x, -y+3/2, z+1/2.

Table S6. Hydrogen bonding parameters for **2**.

D-H...A	d(D-H) (Å)	d(H...A) (Å)	d(D...A)(Å)	<(D-H...A) (°)
C(12)-H(12A)...O(10)#7	0.98	2.48	3.448(4)	170
C(2)-H(2A)...O(5)#9	0.98	2.47	3.379(5)	154.8
C(35)-H(35A)...O(10)	0.93	2.38	3.255(5)	157.8
C(36)-H(36A)...O(3W)	0.93	2.6	3.065(5)	111.7
N(1)-H(1C)...O(7)	0.91	2.29	3.138(4)	155.3
N(2)-H(2B)...O(3)	0.91	2.25	3.089(4)	152.6
O(1W)-H(1WA)...O(5)#9	0.85	2.11	2.775(4)	134.6
O(1W)-H(1WB)...O(5W)	0.85	2.05	2.788(4)	144.6
O(2W)-H(2WA)...O(10)#7	0.85	2.06	2.728(4)	135.3
O(2W)-H(2WB)...O(7W)	0.85	2.28	2.789(4)	118.5
O(3W)-H(3WA)...O(6)#3	0.85	2.03	2.668(3)	131.2
O(3W)-H(3WB)...O(5)#3	0.85	2.12	2.966(4)	176.1
O(4W)-H(4WA)...O(10)	0.85	2.59	3.385(4)	156.3
O(4W)-H(4WB)...O(1)	0.85	2.21	2.674(3)	114.3
O(5W)-H(5WA)...O(2)	0.85	2.07	2.839(4)	150.7
O(5W)-H(5WB)...O(4)#9	0.85	2.54	3.023(4)	117.1
O(6W)-H(6WA)...O(3)	0.85	2.03	2.868(4)	170.7
O(7W)-H(7WA)...O(8)	0.85	2	2.776(4)	150.4
O(7W)-H(7WB)...O(8W)#8	0.85	2.42	2.831(5)	110.7
O(8W)-H(8WA)...O(10)#7	0.85	2.06	2.688(4)	130.2
O(9W)-H(9WA)...N(6)#2	0.85	2.59	3.417(5)	164.9

Symmetry codes: #1: x+1, y, z-1; #2: x-1, y, z; #3: x, y, z+1; #4: x-1, y, z+1; #5: x+1, y, z; #6: x, y, z-1; #7: -x+1, -y+1, -z+1; #8: -x+1, -y+1, -z; #9: x, -y+3/2, z+1/2.

Table S7. Hydrogen bonding parameters for **3**.

D-H...A	d(D-H) (Å)	d(H...A) (Å)	d(D...A)(Å)	<(D-H...A) (°)
C(1)-H(1B)...O(1W)	0.97	2.61	3.121(4)	113.3
N(1)-H(1)...O(1)#1	0.98	2.74	3.005(3)	96.1
N(1)-H(1)...O(3)#1	0.98	2.25	3.160(3)	154.2
O(1W)-H(1WA)...O(5)#10	0.85	1.97	2.788(3)	161.8
O(1W)-H(1WB)...O(4W)#9	0.85	2.03	2.847(3)	160.4
O(2W)-H(2WA)...O(1)	0.85	1.87	2.688(3)	160.5
O(2W)-H(2WB)...O(4W)#8	0.85	2.05	2.749(4)	139
O(3W)-H(3WA)...O(5)#7	0.85	2.27	3.085(4)	162
O(3W)-H(3WB)...O(3)#6	0.85	2	2.844(3)	173.9
O(4W)-H(4WA)...O(2)#1	0.85	1.88	2.708(3)	163.9
O(4W)-H(4WB)...O(4)#5	0.85	2.01	2.759(3)	146.3

Symmetry codes: #1: -x+2, -y+1, -z+1; #2: x+1, y-1, z; #3: -x+2, -y+2, -z+1; #4: x-1, y+1, z; #5: x, -y+1/2, z+1/2; #6: x-1, y, z; #7: -x+1, y+1/2, -z+1/2; #8: x, y+1, z; #9: x, -y+1/2, z-1/2; #10: -x+2, y+1/2, -z+1/2.

Table S8 Hydrogen bonding parameters for **4**.

D-H...A	d(D-H) (Å)	d(H...A) (Å)	d(D...A) (Å)	<(D-H...A) (°)
O(2W)-H(2WA)...O(1W)#3	0.85	2.05	2.87(2)	162.1
O(1W)-H(1WB)...O(5)#4	0.85	2.38	3.107(12)	143.6
O(1W)-H(1WB)...O(4)#4	0.85	2.27	3.029(10)	149.4
O(1W)-H(1WA)...O(5)	0.85	2.39	2.892(15)	118.7
N(1)-H(1C)...O(1)#1	0.9	2.5	3.215(9)	137.3
C(23)-H(23)...O(5)#5	0.93	2.45	3.311(10)	154.9

Symmetry codes: #1 -x+2, -y, -z; #2 -x+2, y, -z+1/2; #3 x, y+1, z; #4 -x+3/2, -y+1/2, -z; #5 x+1/2, -y+1/2, z+1/2.

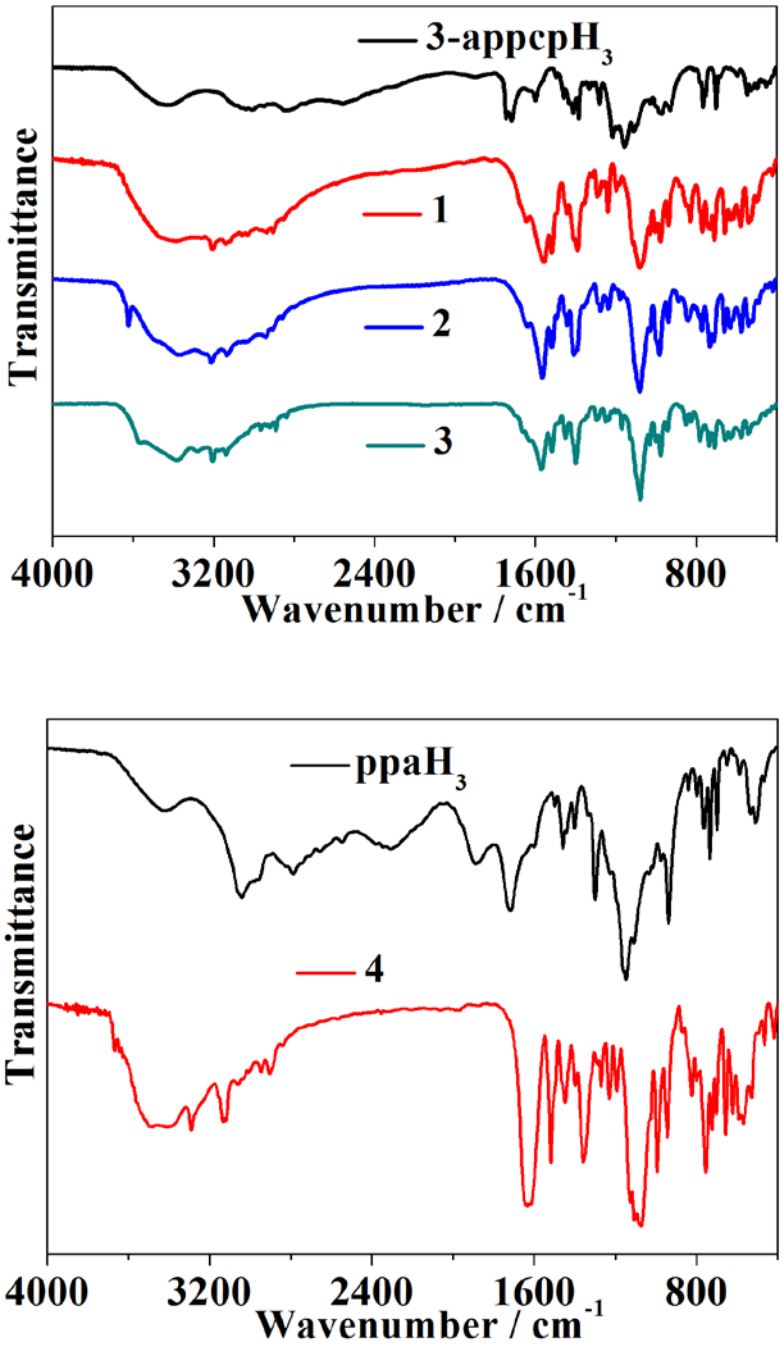

Fig. S1. The IR spectra for compounds **3-ppapH$_3$, ppaH$_3$** and **1-4**.

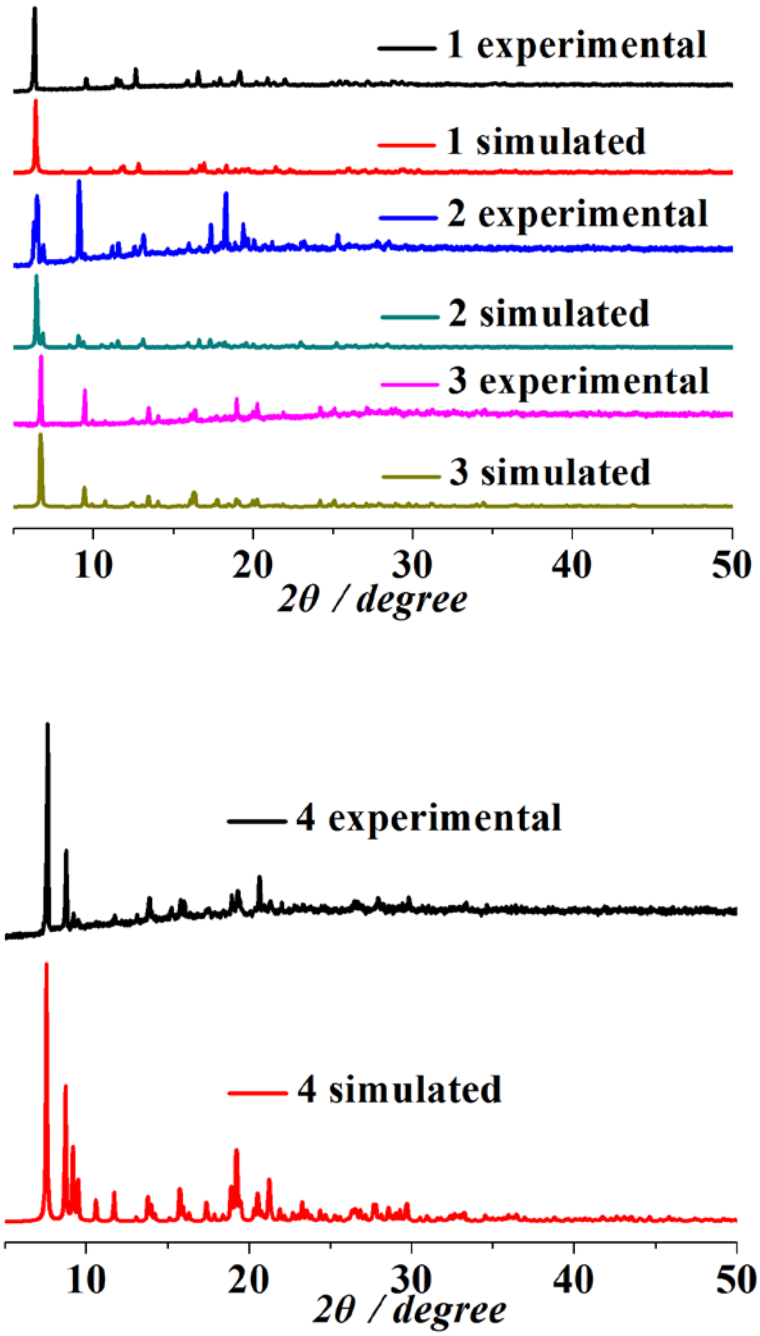

Fig. S2. XRD patterns for compounds **1-4**.

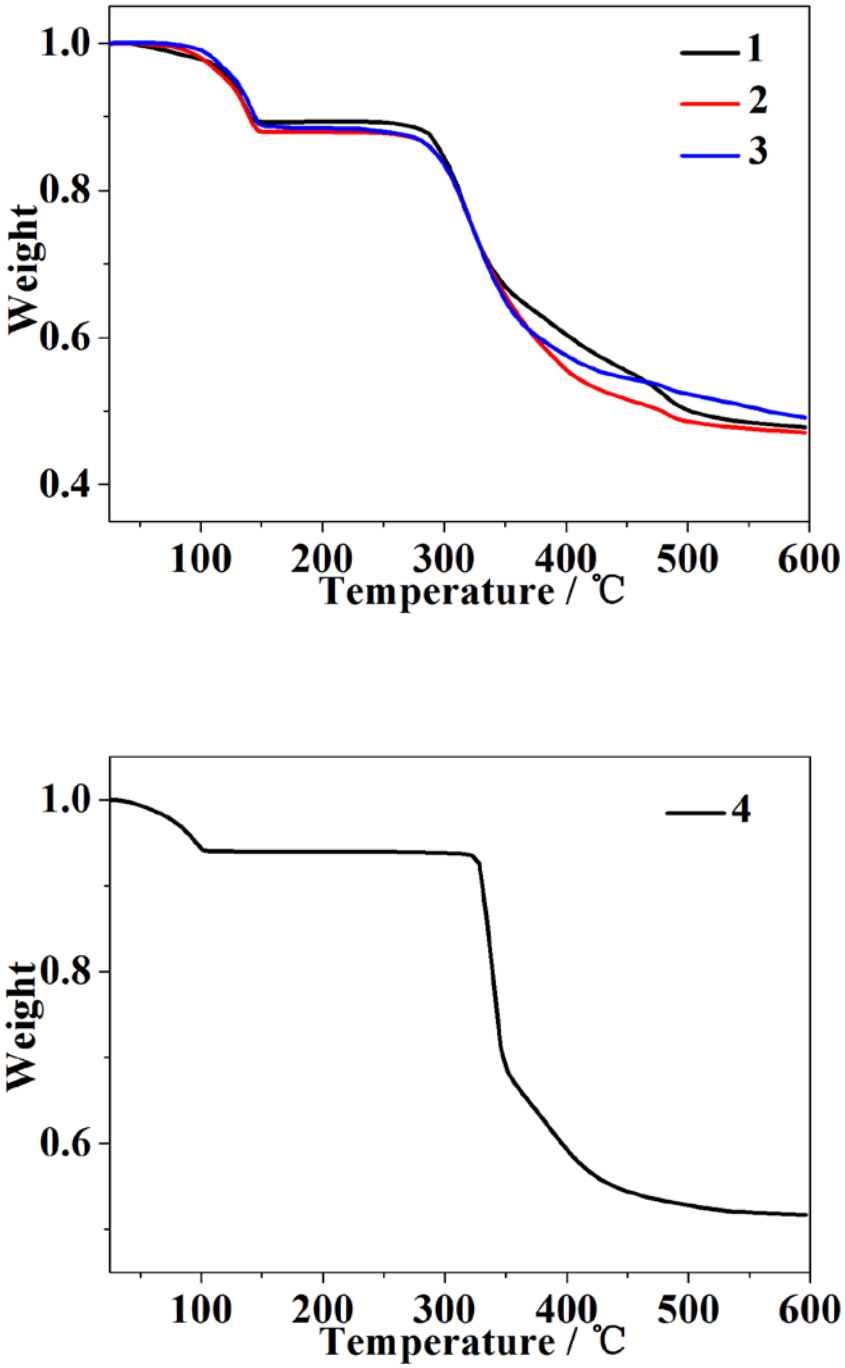

Fig. S3. TGA curves for compounds **1-4**.

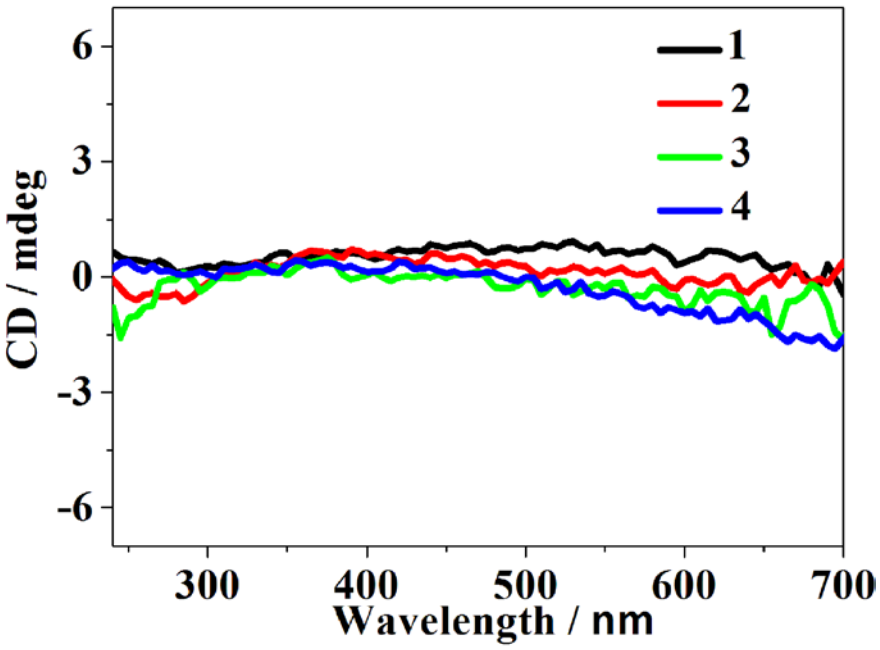

Fig. S4. CD spectra for compounds **1-4**.

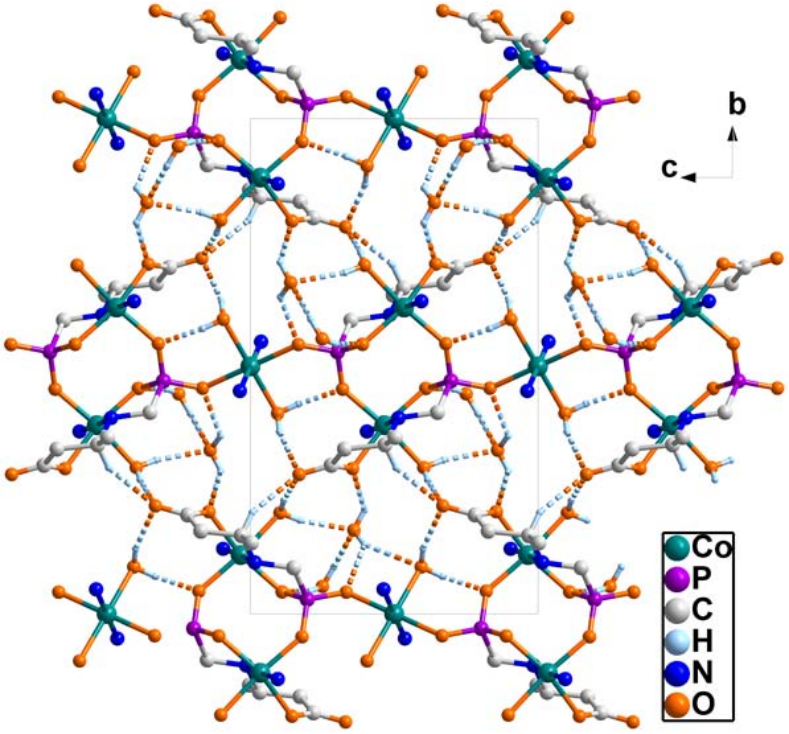

Fig. S5. The hydrogen bond network in compound **1**.

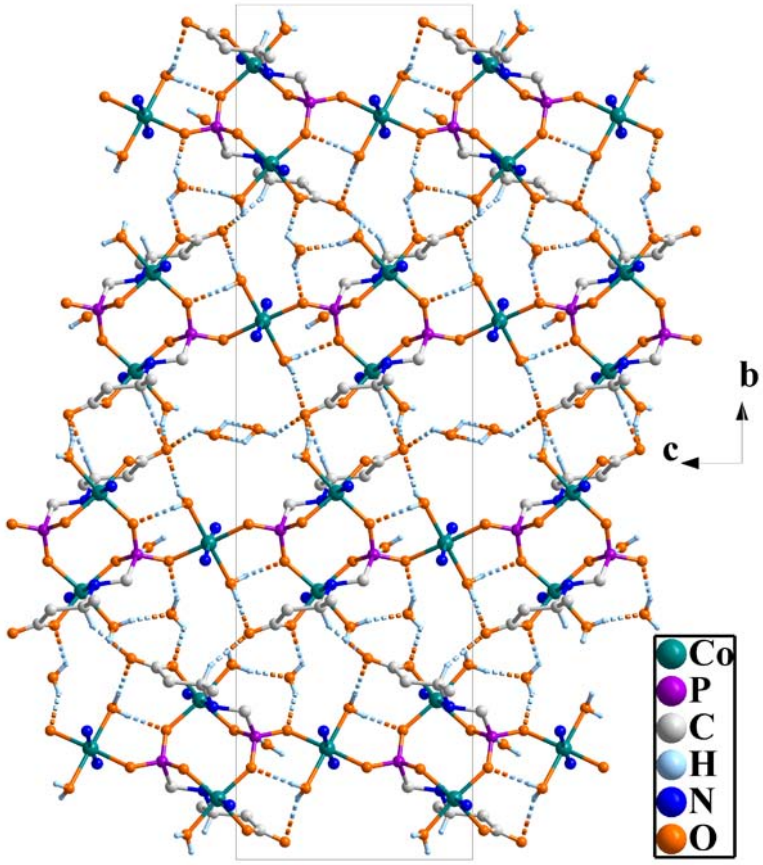

Fig. S6. The hydrogen bond network in compound **2**.

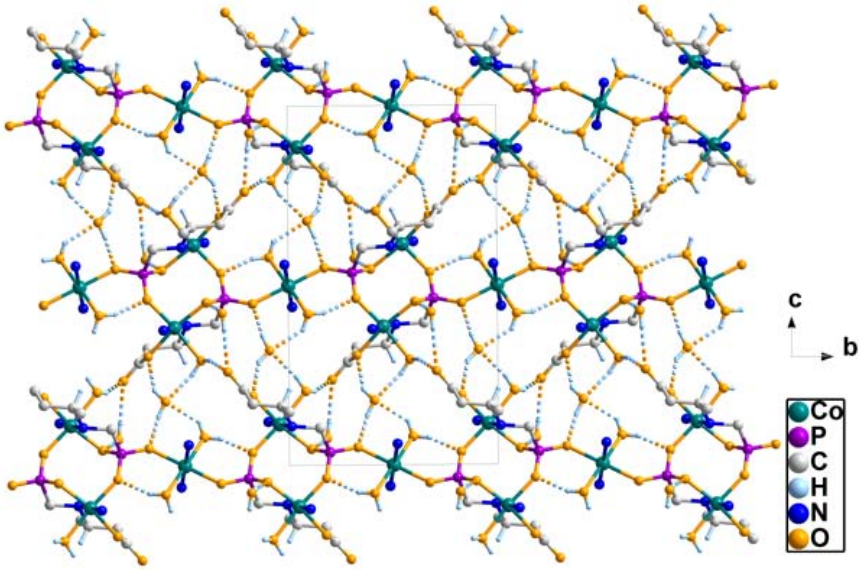

Fig. S7. The hydrogen bond network in compound **3**.

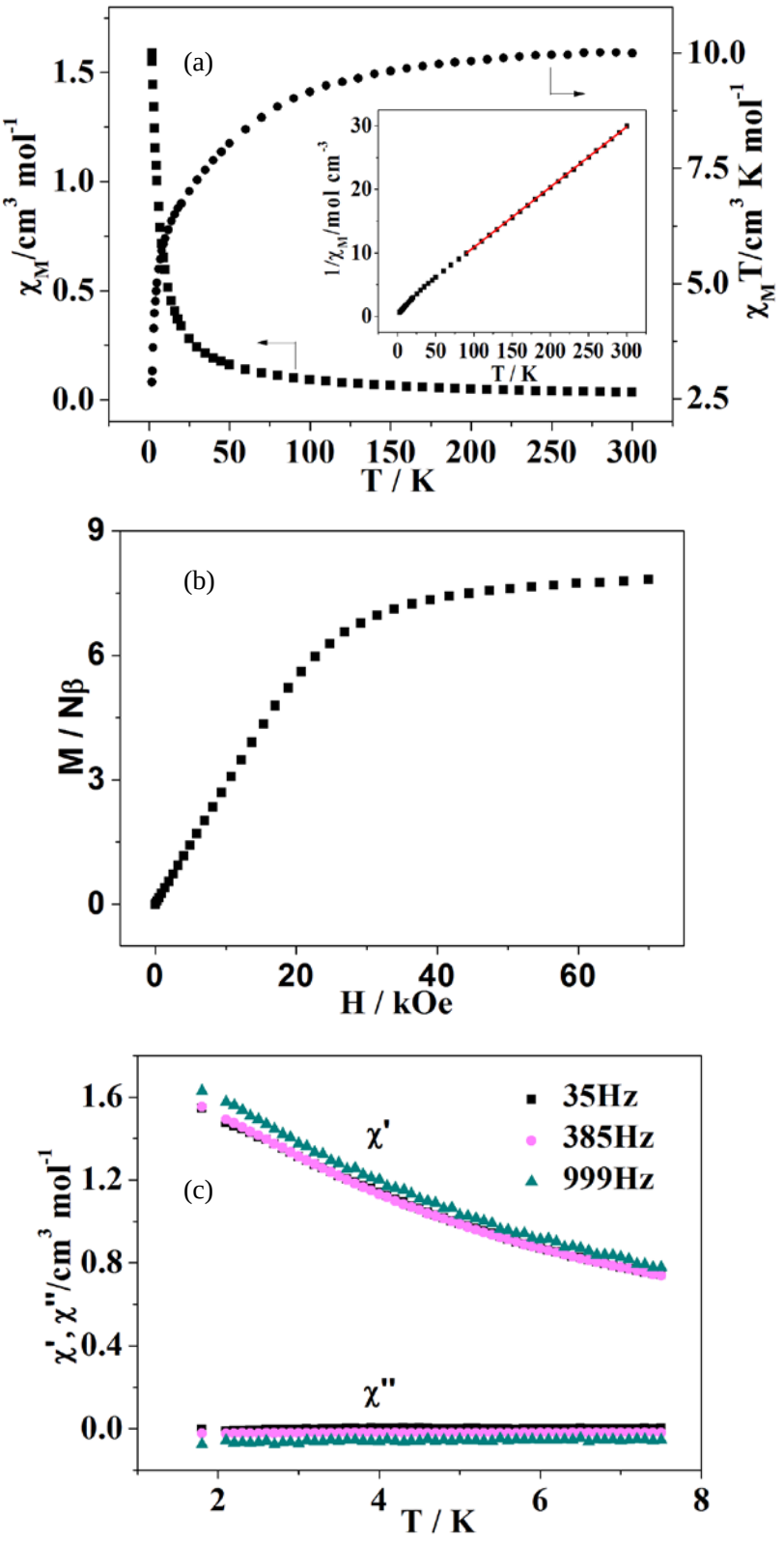

Fig. S8 The χ_M, $\chi_M T$, $1/\chi_M$ vs. T (a), M vs. H at 1.8 K (b) and χ' and χ'' vs. T (c) plots for compound **1**.

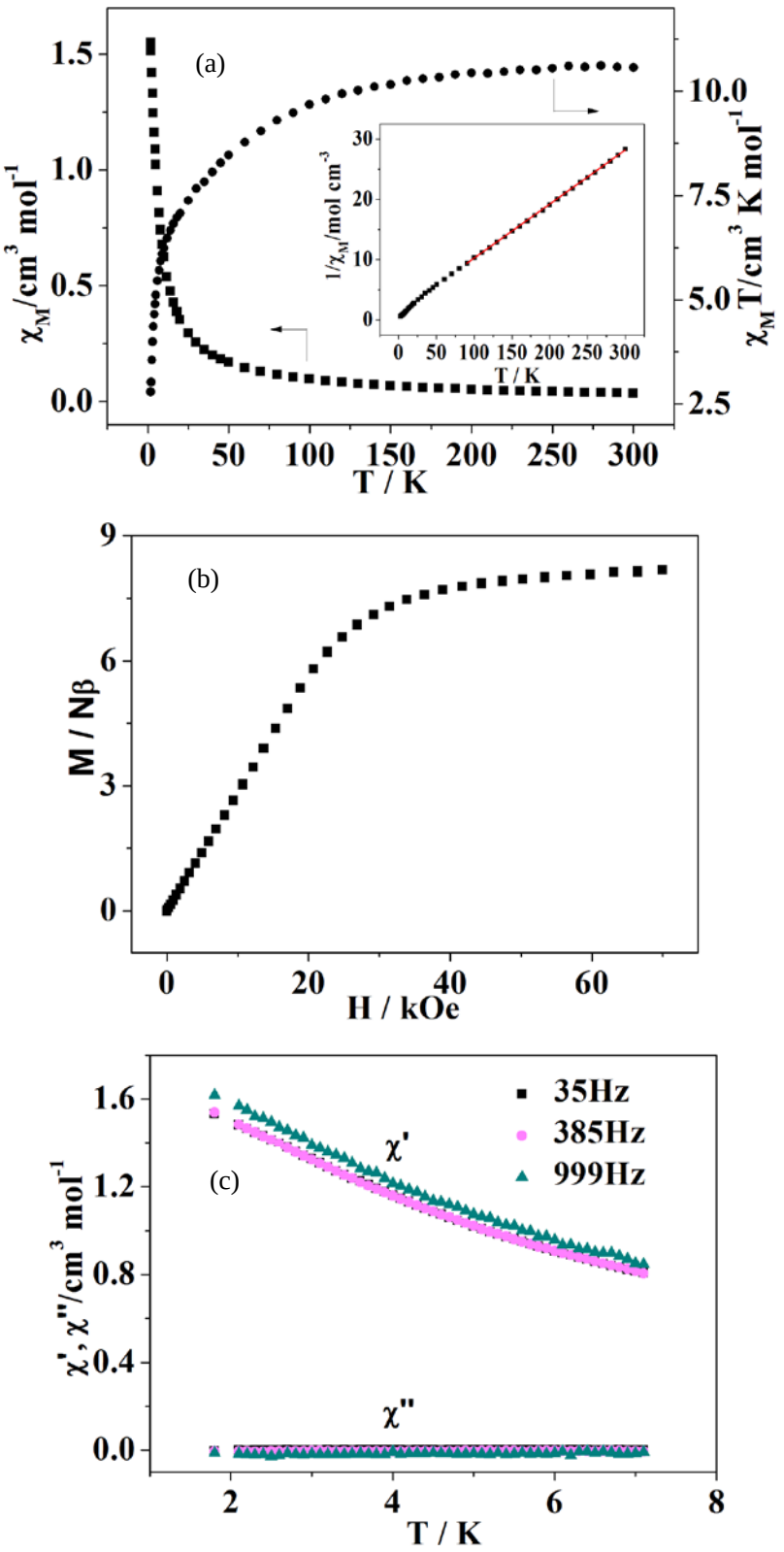

Fig. S9 The χ_M, $\chi_M T$, $1/\chi_M$ vs. T (a), M vs. H at 1.8 K (b) and χ' and χ'' vs. T (c) plots for compound **2**.

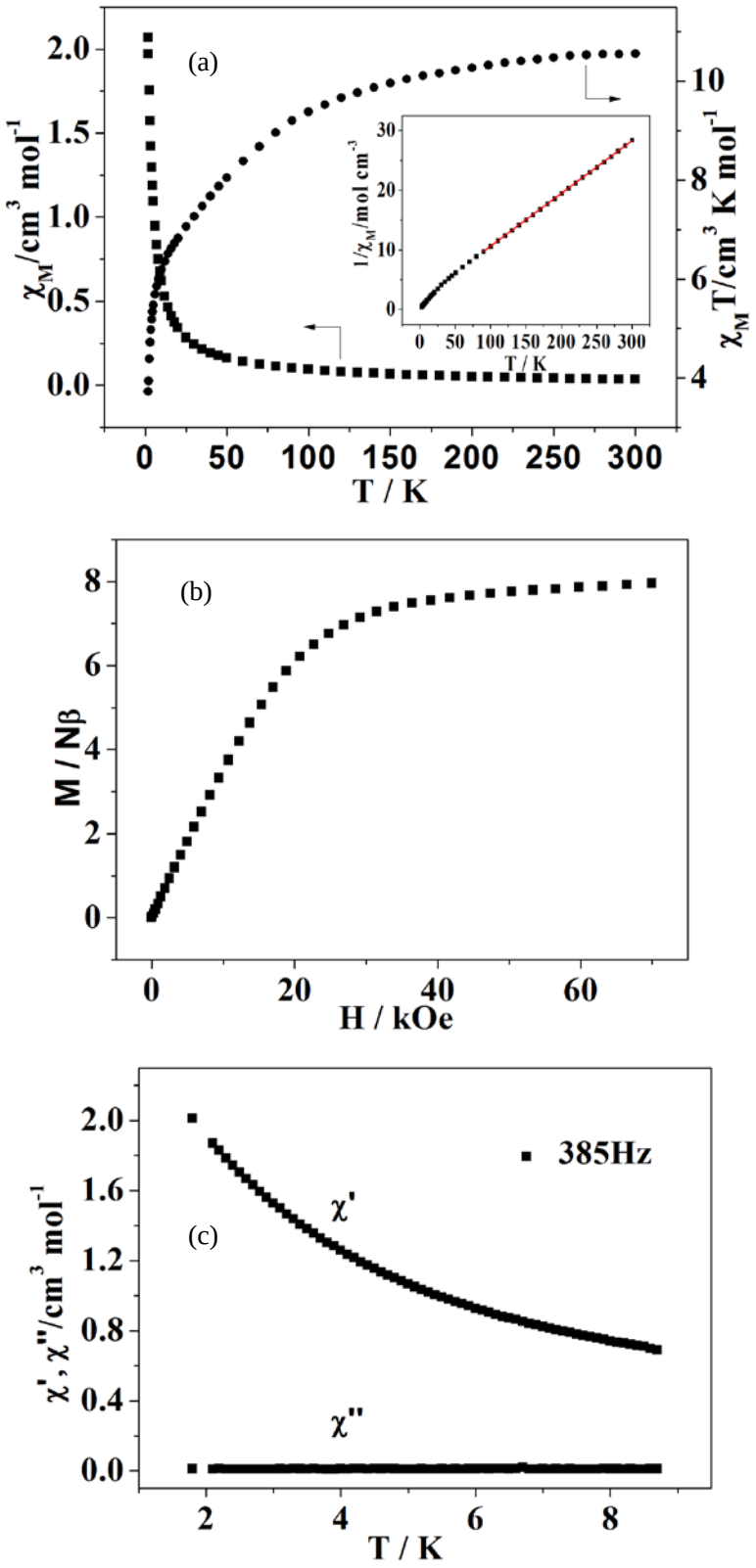

Fig. S10 The χ_M, $\chi_M T$, $1/\chi_M$ vs. T (a), M vs. H at 1.8 K (b) and χ' and χ'' vs. T (c) plots for compound **3**.

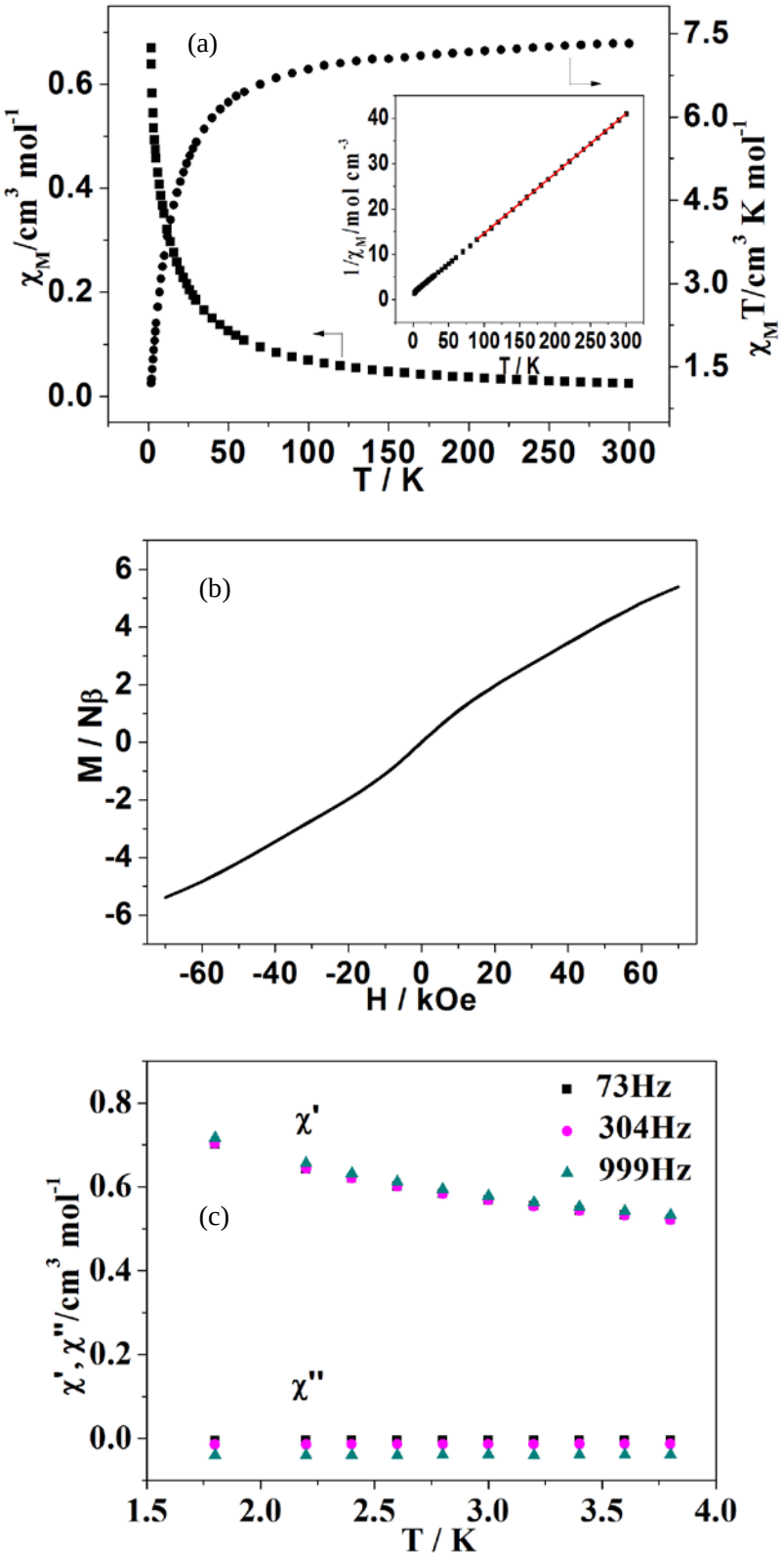

Fig. S11 The χ_M, $\chi_M T$, $1/\chi_M$ vs. *T* (a), M vs. *H* at 1.8 K (b) and χ' and χ'' vs. *T* (c) plots for compound **4**.