Supplementary Information

Butterfly-like enantiomerically homochiral $\{Co^{II}_6Co^{III}_4\}$ clusters exhibiting both slow magnetic relaxation and ferroelectric property

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X-ray Crystallography

The disorder of perchlorates and one of the hydroxide ions have been treated as follows:

First of all, the four ClO_4^- anions in ***S*-1** and ***R*-1** are heavily disordered. All the oxygen atoms in each ClO_4^- anion were split into two parts with refined occupancies. For ***S*-1**, the refined occupancies are 0.665(17) and 0.335(17) for those attached to Cl(1), 0.395(11) and 0.605(11) for those attached to Cl(2), 0.759(9) and 0.241(9) for those attached to Cl(3), and 0.539(6) and 0.461(6) for those attached to Cl(4) and Cl(4B), respectively. For ***R*-1**, the refined occupancies are 0.694(9) and 0.306(9) for those attached to Cl(1), 0.669(19) and 0.331(19) for those attached to Cl(2), 0.459(12) and 0.541(12) for those attached to Cl(3) and Cl(3B), and 0.535(5) and 0.465(5) for those attached to Cl(4) and Cl(4B), respectively. Note that some of the Cl atoms (Cl(3)/Cl(3B) in ***R*-1** and Cl(4)/Cl(4B) in both structures) in the ClO_4 were also split into two sets with corresponding refined occupancies (Fig. S1 and Table S4†).

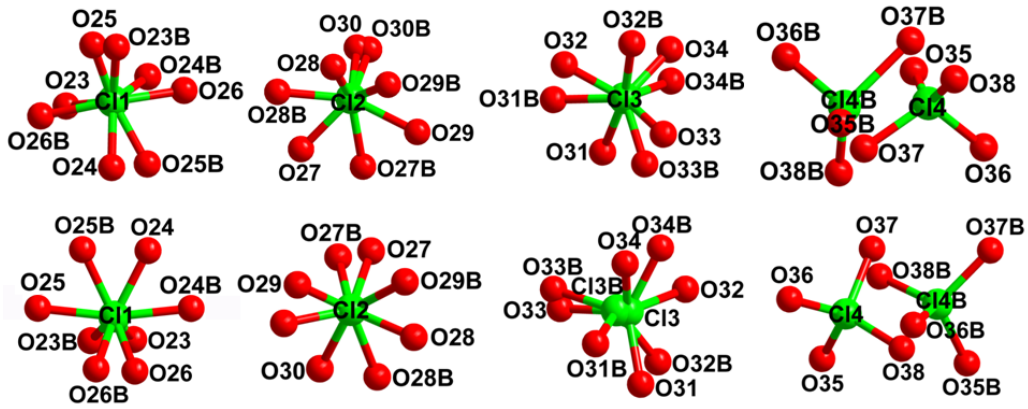


Fig. S1 The four heavily disordered ClO_4^- anions in ***S*-1** (up) and ***R*-1** (down).

Secondly, there both exist a statistical distribution of OH^- and $(OCH_3)^-$ in ***S*-1** and ***R*-1**, that is, both the SOFs of O(22)-H and O(22)-C(93)H_3 were determined to be 0.5. In fact, we refined it as a whole OH group for O(22), but there was always an extra peak (height of 2.0 $eÅ^{-3}$ in ***S*-1** and that slightly lower in ***R*-1**) in the D-F maps which are ~1.65 Å far from O(22). If we considered the peak as a C atom (C93) of a whole OMe^- group, its *U*eq would become extremely large. Finally, the SOF of 0.5 was assigned to C(93) so that a relatively reasonable *U*eq was reached for C(93). (Fig. S2a

and S2b, and Table S4†). Accordingly the SOF of one of the lattice water molecules (O(3W)) was reduced to 0.5, as it formed a hydrogen bond to the half-occupied O(22)H group. Assuming that O(3W) has a SOF of 1.0, the distances between O(3W) and a hydrogen attached to C(93) would be ~1.63 Å, which is unreasonable. In other words, the O(22)H and O(3W)H_2 having SOFs of 0.5, are statistical distributed with O(22)C(93)H_3 group that have SOF of 0.5 in both ***S*-1** and ***R*-1** (Fig. S2c†)

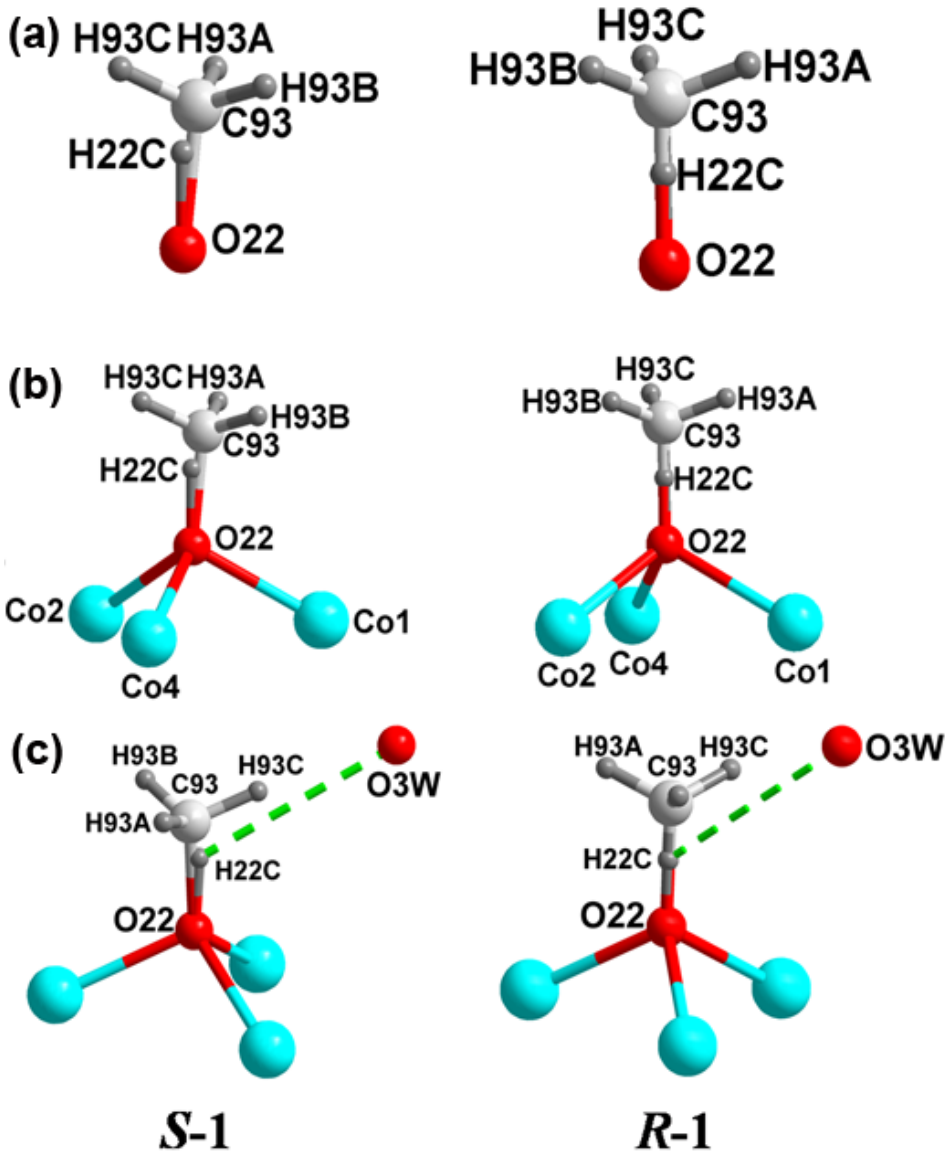


Fig. S2 (a) and (b) The statistical distribution of OH^- and $(OCH_3)^-$ in ***S*-1** and ***R*-1**. (c) The hydrogen bonding interaction of O(3W) and O(22)H in ***S*-1** and ***R*-1**.

Thirdly, some other guest water molecules also underwent vacancy disordering in ***S*-1** and ***R*-1**. Due to the splitting of the $Cl(4)O_4$ and $Cl(4B)O_4$ groups in ***S*-1**, the O(4W) and O(5W) exhibited vacancy disordering with the occupancy reduced to 0.270(3) and 0.230(3), respectively; otherwise the *U*eq of O(4W) and O(5W) are very high. Similarly, the SOF of O(6W) in ***S*-1** was assigned to 0.5. As for ***R*-1**, the SOFs of O(4W) and O(5W) were 0.535(5) and 0.465(5), respectively (Table S4†). To summarize, ***S*-1** and ***R*-1** both contain three and a half lattice water molecules: O(1W)(1), O(2W)(1), O(3W)(0.5), O(4W)(0.270(3)), O(5W)(0.230(3)) and O(6W)(0.5) for ***S*-1** and O(1W)(1), O(2W)(1), O(3W)(0.5), O(4W)(0.535(5)) and O(5W)(0.465(5)) for ***R*-1**, respectively, which also can be confirmed by the TGA results (Fig. S7†).

Finally, analyses of the bond lengths, charge balance and bond valence sum calculations (BVS)[1] suggest that Co5, Co6, Co8 and Co9 are assigned the oxidation state of +3, whereas Co1, Co2, Co3, Co4, Co7 and Co10 are assigned oxidation state of +2 (Table S3†). In addition, based on the (BVS) calculations, the values of the μ_1-O atoms from the $pdmH_2$ ligands are O1(0.578), O3(0.289), O10(0.304) and O11(0.573) for ***S*-1** and O1(0.521), O3(0.295), O10(0.311) and O11(0.635) for ***R*-1**, respectively (Table S3†). It suggests that the methanol groups associated with O3 and O10 have not been deprotonated while those with O1 and O11 are deprotonated in both ***S*-1** and ***R*-1** (Fig. S3†).[2]

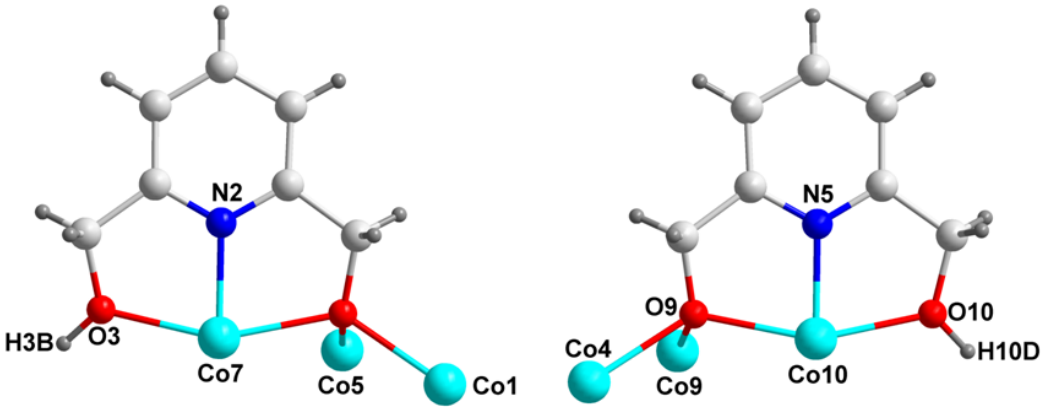
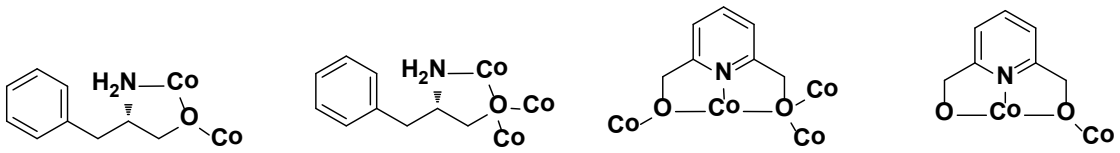


Fig. S3 The μ_1-OH atoms from the $pdmH^-$ ligands in ***S*-1.**

Based on the above considerations, complexes ***S*-1** and ***R*-1** can be formulated as $[Co^{II}_6Co^{III}_4(\mu_3\text{-OH})(\mu_3\text{-X})(S\text{-pa})_4(pdm)_6(pdmH)_2](ClO_4)_4\cdot 3.5H_2O$ (***S*-1**) and $[Co^{II}_6Co^{III}_4(\mu_3\text{-OH})(\mu_3\text{-X})(R\text{-pa})_4(pdm)_6(pdmH)_2](ClO_4)_4\cdot 3.5H_2O$ (***R*-1**) (X = OH or OMe). Crystallographic data and other pertinent information are summarized in Table S1†.

Reference

1. (a) N. E. Brese and M. O'Keeffe, *Acta Crystallogr.*, 1991, **B47**, 192;
   (b) I. D. Brown and D. Altermatt, *Acta Crystallogr.*, 1985, **B41**, 244.
2. M. Wang, D. Q. Yuan, C. B. Ma, M. J. Yuan, M. Q. Hu, N. Li, H. Chen, C. N. Chen and Q. T. Liu, *Dalton Trans.*, 2010, **39**, 7276.



[2.21] **[3.31]** **[4.321]** **[2.211]**

Scheme S1 The coordination modes of *S*-paH and $pdmH_2$ ligands.

Table S1 Crystallographic data for compounds ***S*-1** and ***R*-1**

Compound	***S*-1**	***R*-1**
CCDC	950149	950150
Formula	$C_{92.5}H_{109}Co_{10}N_{12}O_{22}\cdot 4(ClO_4)\cdot 3.5(H_2O)$	$C_{92.5}H_{109}Co_{10}N_{12}O_{22}\cdot 4(ClO_4)\cdot 3.5(H_2O)$
Formula mass	2791.07	2791.07
Crystal system	monoclinic	monoclinic
Space group	$P2_1$	$P2_1$
a (Å)	15.033(7)	15.130(8)
b (Å)	25.599(11)	25.739(12)
c (Å)	15.034(7)	15.205(7)
α (°)	90	90
β (°)	107.686(7)	107.966(9)
γ (°)	90	90
V (Å^3)	5512(4)	5633(5)
Z	2	2
μ (mm^{-1})	1.652	1.617
D_{calcd} (g/cm^3)	1.682	1.646
F(000)	2850.0	2850.0
R_1[a] [$I>2\sigma(I)$]	0.0541	0.0647
wR_2[b] [$I>2\sigma(I)$]	0.1353	0.1306
GOF on F^2	1.006	1.004
Flack parameter	-0.0041	0.0159

[a] $R_1 = \sum \| F_o | - | F_c \| / \sum | F_o |$, [b] $wR_2 = [\sum w(F_o^2 - F_c^2)^2 / \sum w(F_o^2)^2]^{0.5}$

Table S2 Bond lengths (Å) and angles (º) for complexes ***S*-1** and ***R*-1**.

***S*-1**			
Co1—O8	1.984 (4)	Co6—N6	1.842 (6)
Co1—O22	2.038 (3)	Co6—O18	1.891 (4)
Co1—O21	2.126 (4)	Co6—O11	1.893 (5)
Co1—O5	2.173 (4)	Co6—O12	1.923 (5)
Co1—O4	2.181 (4)	Co6—N10	1.939 (5)
Co1—O17	2.188 (4)	Co6—O14	1.949 (4)
Co1—Co5	2.7304 (14)	Co6—Co7	2.9967 (15)
Co2—N7	2.048 (5)	Co7—O18	2.001 (4)
Co2—O13	2.052 (4)	Co7—N2	2.012 (6)
Co2—O22	2.058 (4)	Co7—O6	2.068 (4)
Co2—O12	2.129 (4)	Co7—O14	2.099 (4)
Co2—O14	2.160 (4)	Co7—O3	2.143 (5)
Co2—O17	2.209 (4)	Co7—O4	2.220 (4)
Co3—O8	2.038 (4)	Co8—N1	1.850 (5)
Co3—N4	2.047 (5)	Co8—O20	1.891 (4)
Co3—O21	2.049 (4)	Co8—O1	1.895 (5)
Co3—O2	2.152 (4)	Co8—N12	1.927 (5)
Co3—O7	2.166 (4)	Co8—O2	1.935 (4)
Co3—O19	2.185 (4)	Co8—O7	1.961 (4)
Co4—O13	2.008 (4)	Co9—N8	1.825 (5)
Co4—O21	2.036 (3)	Co9—O15	1.894 (4)
Co4—O15	2.084 (4)	Co9—O16	1.904 (4)
Co4—O22	2.100 (4)	Co9—O19	1.931 (4)
Co4—O9	2.213 (4)	Co9—N11	1.940 (5)
Co4—O19	2.284 (4)	Co9—O9	1.948 (4)
Co4—Co9	2.7295 (14)	Co9—Co10	2.9957 (15)
Co5—N3	1.820 (5)	Co10—N5	2.008 (5)
Co5—O5	1.902 (4)	Co10—O20	2.053 (4)
Co5—O6	1.911 (4)	Co10—O7	2.075 (4)
Co5—N9	1.925 (5)	Co10—O16	2.100 (4)
Co5—O17	1.928 (4)	Co10—O10	2.140 (4)
Co5—O4	1.951 (4)	Co10—O9	2.182 (4)
O8—Co1—O22	103.62 (16)	O14—Co2—O17	88.98 (14)
O8—Co1—O21	82.30 (16)	O8—Co3—N4	78.27 (18)
O22—Co1—O21	81.92 (14)	O8—Co3—O21	82.95 (15)

O8—Co1—O5	98.66 (16)	N4—Co3—O21	161.01 (18)
O22—Co1—O5	157.15 (15)	O8—Co3—O2	100.33 (16)
O21—Co1—O5	106.28 (14)	N4—Co3—O2	95.74 (17)
O8—Co1—O4	111.59 (16)	O21—Co3—O2	90.40 (15)
O22—Co1—O4	90.33 (14)	O8—Co3—O7	154.83 (15)
O21—Co1—O4	165.47 (14)	N4—Co3—O7	77.19 (17)
O5—Co1—O4	76.68 (14)	O21—Co3—O7	121.77 (15)
O8—Co1—O17	171.31 (16)	O2—Co3—O7	76.70 (15)
O22—Co1—O17	83.65 (14)	O8—Co3—O19	99.62 (15)
O21—Co1—O17	94.19 (15)	N4—Co3—O19	96.13 (16)
O5—Co1—O17	74.62 (14)	O21—Co3—O19	84.11 (14)
O4—Co1—O17	72.65 (14)	O2—Co3—O19	158.47 (15)
O8—Co1—Co5	133.09 (12)	O7—Co3—O19	88.53 (14)
O22—Co1—Co5	114.35 (11)	O13—Co4—O21	103.14 (17)
O21—Co1—Co5	128.02 (11)	O13—Co4—O15	99.41 (16)
O5—Co1—Co5	43.83 (11)	O21—Co4—O15	155.99 (16)
O4—Co1—Co5	45.11 (10)	O13—Co4—O22	83.20 (15)
O17—Co1—Co5	44.49 (10)	O21—Co4—O22	82.62 (14)
N7—Co2—O13	77.88 (18)	O15—Co4—O22	108.33 (15)
N7—Co2—O22	160.30 (17)	O13—Co4—O9	111.01 (16)
O13—Co2—O22	83.18 (15)	O21—Co4—O9	87.17 (14)
N7—Co2—O12	98.04 (18)	O15—Co4—O9	77.09 (15)
O13—Co2—O12	102.08 (17)	O22—Co4—O9	164.16 (14)
O22—Co2—O12	91.12 (15)	O13—Co4—O19	174.78 (15)
N7—Co2—O14	76.68 (17)	O21—Co4—O19	81.94 (14)
O13—Co2—O14	153.94 (15)	O15—Co4—O19	75.75 (14)
O22—Co2—O14	122.64 (15)	O22—Co4—O19	96.38 (14)
O12—Co2—O14	76.08 (15)	O9—Co4—O19	70.11 (14)
N7—Co2—O17	94.81 (17)	O13—Co4—Co9	132.91 (12)
O13—Co2—O17	98.75 (15)	O21—Co4—Co9	112.70 (11)
O22—Co2—O17	82.68 (14)	O15—Co4—Co9	43.84 (11)
O12—Co2—O17	157.40 (16)	O22—Co4—Co9	129.60 (11)
O9—Co4—Co9	44.92 (10)	O11—Co6—O14	91.69 (19)
O19—Co4—Co9	44.19 (9)	O12—Co6—O14	86.10 (16)
N3—Co5—O5	86.21 (19)	N10—Co6—O14	166.0 (2)
N3—Co5—O6	85.4 (2)	N6—Co6—Co7	137.97 (17)
O5—Co5—O6	171.09 (16)	O18—Co6—Co7	41.00 (13)

N3—Co5—N9	94.1 (2)	O11—Co6—Co7	81.51 (15)
O5—Co5—N9	91.3 (2)	O12—Co6—Co7	104.80 (11)
O6—Co5—N9	92.4 (2)	N10—Co6—Co7	122.62 (18)
N3—Co5—O17	173.5 (2)	O14—Co6—Co7	44.20 (12)
O5—Co5—O17	87.29 (16)	O18—Co7—N2	97.4 (2)
O6—Co5—O17	101.03 (16)	O18—Co7—O6	164.04 (17)
N9—Co5—O17	86.69 (18)	N2—Co7—O6	97.85 (19)
N3—Co5—O4	95.50 (19)	O18—Co7—O14	75.15 (16)
O5—Co5—O4	89.01 (17)	N2—Co7—O14	170.49 (19)
O6—Co5—O4	88.75 (17)	O6—Co7—O14	90.17 (15)
N9—Co5—O4	170.35 (18)	O18—Co7—O3	95.44 (19)
O17—Co5—O4	83.69 (16)	N2—Co7—O3	78.6 (2)
N3—Co5—Co1	121.99 (15)	O6—Co7—O3	92.25 (18)
O5—Co5—Co1	52.31 (11)	O14—Co7—O3	96.05 (18)
O6—Co5—Co1	131.15 (12)	O18—Co7—O4	100.44 (16)
N9—Co5—Co1	121.25 (17)	N2—Co7—O4	78.47 (19)
O17—Co5—Co1	52.67 (12)	O6—Co7—O4	77.98 (15)
O4—Co5—Co1	52.36 (12)	O14—Co7—O4	108.37 (15)
N6—Co6—O18	178.5 (2)	O3—Co7—O4	153.53 (18)
N6—Co6—O11	84.1 (3)	O18—Co7—Co6	38.32 (12)
O18—Co6—O11	96.6 (2)	N2—Co7—Co6	130.58 (16)
N6—Co6—O12	84.4 (2)	O6—Co7—Co6	129.22 (11)
O18—Co6—O12	94.86 (19)	O14—Co7—Co6	40.35 (10)
O11—Co6—O12	167.9 (2)	O3—Co7—Co6	84.65 (15)
N6—Co6—N10	96.6 (2)	O4—Co7—Co6	120.62 (10)
O18—Co6—N10	84.8 (2)	N1—Co8—O20	178.3 (2)
O11—Co6—N10	90.2 (2)	N1—Co8—O1	84.6 (2)
O12—Co6—N10	94.8 (2)	O20—Co8—O1	96.3 (2)
N6—Co6—O14	97.4 (2)	N1—Co8—N12	94.5 (2)
O18—Co6—O14	81.27 (17)	O20—Co8—N12	87.0 (2)
O1—Co8—N12	88.5 (2)	N11—Co9—Co10	132.62 (17)
N1—Co8—O2	84.3 (2)	O9—Co9—Co10	46.68 (11)
O20—Co8—O2	94.78 (18)	Co4—Co9—Co10	90.36 (3)
O1—Co8—O2	168.7 (2)	N5—Co10—O20	97.18 (19)
N12—Co8—O2	94.6 (2)	N5—Co10—O7	168.36 (19)
N1—Co8—O7	97.6 (2)	O20—Co10—O7	74.63 (15)
O20—Co8—O7	81.00 (16)	N5—Co10—O16	95.71 (18)

O1—Co8—O7	92.38 (18)	O20—Co10—O16	165.02 (17)
N12—Co8—O7	168.0 (2)	O7—Co10—O16	93.62 (15)
O2—Co8—O7	86.89 (16)	N5—Co10—O10	78.4 (2)
N8—Co9—O15	86.4 (2)	O20—Co10—O10	96.82 (18)
N8—Co9—O16	85.5 (2)	O7—Co10—O10	94.14 (18)
O15—Co9—O16	171.12 (17)	O16—Co10—O10	93.21 (17)
N8—Co9—O19	175.5 (2)	N5—Co10—O9	79.36 (19)
O15—Co9—O19	89.21 (16)	O20—Co10—O9	96.98 (15)
O16—Co9—O19	98.83 (17)	O7—Co10—O9	109.48 (15)
N8—Co9—N11	93.6 (2)	O16—Co10—O9	77.93 (15)
O15—Co9—N11	90.5 (2)	O10—Co10—O9	155.09 (17)
O16—Co9—N11	93.6 (2)	N5—Co10—Co9	95.68 (16)
O19—Co9—N11	87.16 (18)	O20—Co10—Co9	131.39 (12)
N8—Co9—O9	95.56 (19)	O7—Co10—Co9	95.95 (11)
O15—Co9—O9	88.42 (17)	O16—Co10—Co9	39.13 (11)
O16—Co9—O9	88.75 (17)	O10—Co10—Co9	131.70 (13)
O19—Co9—O9	83.53 (16)	O9—Co10—Co9	40.49 (10)
N11—Co9—O9	170.65 (18)	C1—O1—Co8	113.6 (5)
N8—Co9—Co4	120.52 (17)	C1—O1—H1C	123.2
O15—Co9—Co4	49.64 (12)	Co8—O1—H1C	123.2
O16—Co9—Co4	133.14 (12)	C7—O2—Co8	111.7 (4)
O19—Co9—Co4	55.55 (12)	C7—O2—Co3	115.3 (4)
N11—Co9—Co4	119.83 (16)	Co8—O2—Co3	98.01 (16)
O9—Co9—Co4	53.35 (12)	C8—O3—Co7	111.1 (5)
N8—Co9—Co10	101.26 (17)	C14—O4—Co5	125.1 (3)
O15—Co9—Co10	134.73 (13)	C14—O4—Co1	112.0 (3)
O16—Co9—Co10	44.11 (12)	Co5—O4—Co1	82.53 (14)
O19—Co9—Co10	81.32 (12)	C14—O4—Co7	108.7 (3)
Co5—O4—Co7	91.84 (16)	Co4—O21—Co3	102.81 (17)
Co1—O4—Co7	133.62 (17)	Co4—O21—Co1	97.36 (15)
C15—O5—Co5	112.5 (3)	Co3—O21—Co1	94.94 (16)
C15—O5—Co1	126.7 (3)	Co4—O21—H21C	119.0
Co5—O5—Co1	83.87 (14)	Co3—O21—H21C	119.0
C21—O6—Co5	111.1 (4)	Co1—O21—H21C	119.0
C21—O6—Co7	118.3 (4)	C93—O22—Co1	113.2 (4)
Co5—O6—Co7	97.88 (17)	C93—O22—Co2	123.1 (5)
C22—O7—Co8	121.5 (3)	Co1—O22—Co2	101.39 (16)

C22—O7—Co10	121.6 (3)	C93—O22—Co4	121.2 (5)
Co8—O7—Co10	96.77 (17)	Co1—O22—Co4	98.11 (15)
C22—O7—Co3	111.1 (3)	Co2—O22—Co4	95.24 (16)
Co8—O7—Co3	96.71 (15)	C93—O22—H22C	6.0
Co10—O7—Co3	105.43 (16)	Co1—O22—H22C	119.2
C28—O8—Co1	142.4 (4)	Co2—O22—H22C	119.1
C28—O8—Co3	117.5 (4)	Co4—O22—H22C	119.1
Co1—O8—Co3	99.78 (17)	O22—C93—H22C	11.7
C29—O9—Co9	124.2 (3)	O22—C93—H93A	109.5
C29—O9—Co10	109.2 (3)	O22—C93—H93B	109.5
Co9—O9—Co10	92.83 (16)	H93A—C93—H93B	109.5
C29—O9—Co4	110.3 (3)	O22—C93—H93C	109.5
Co9—O9—Co4	81.74 (14)	H93A—C93—H93C	109.5
Co10—O9—Co4	135.35 (18)	H93B—C93—H93C	109.5
C35—O10—Co10	112.2 (4)	C6—N1—C2	123.6 (6)
C36—O11—Co6	115.5 (5)	C6—N1—Co8	118.1 (4)
C36—O11—H11D	122.3	C2—N1—Co8	118.2 (5)
Co6—O11—H11D	122.3	C9—N2—C13	120.2 (6)
C42—O12—Co6	110.7 (4)	C9—N2—Co7	118.6 (5)
C42—O12—Co2	114.8 (4)	C13—N2—Co7	119.9 (4)
Co6—O12—Co2	99.24 (17)	C16—N3—C20	123.7 (5)
C43—O13—Co4	142.3 (4)	C16—N3—Co5	117.7 (4)
C43—O13—Co2	119.0 (4)	C20—N3—Co5	118.4 (4)
Co4—O13—Co2	98.30 (17)	C23—N4—C27	121.8 (5)
C49—O14—Co6	121.7 (4)	C23—N4—Co3	120.2 (4)
C49—O14—Co7	120.2 (3)	C27—N4—Co3	117.9 (4)
Co6—O14—Co7	95.45 (17)	C34—N5—C30	120.7 (6)
C49—O14—Co2	112.3 (4)	C34—N5—Co10	120.4 (5)
Co6—O14—Co2	97.36 (16)	C30—N5—Co10	118.3 (4)
Co7—O14—Co2	106.34 (16)	C41—N6—C37	124.0 (7)
C50—O15—Co9	111.8 (3)	C41—N6—Co6	118.0 (5)
C50—O15—Co4	128.8 (4)	C37—N6—Co6	118.0 (6)
Co9—O15—Co4	86.52 (15)	C44—N7—Co2	118.3 (4)
C56—O16—Co9	111.3 (4)	C48—N7—Co2	120.2 (4)
C56—O16—Co10	120.4 (4)	C55—N8—Co9	117.8 (4)
Co9—O16—Co10	96.76 (17)	C51—N8—Co9	117.2 (4)
C57—O17—Co5	108.4 (3)	C58—N9—Co5	109.2 (3)

C57—O17—Co1	117.4 (3)	Co5—N9—H9A	109.8
Co5—O17—Co1	82.84 (14)	Co5—N9—H9B	109.8
C57—O17—Co2	114.9 (3)	C67—N10—Co6	104.9 (4)
Co5—O17—Co2	133.22 (19)	Co6—N10—H10C	110.8
Co1—O17—Co2	92.23 (14)	C76—N11—Co9	107.3 (4)
C66—O18—Co6	114.5 (4)	Co9—N11—H11B	110.3
C66—O18—Co7	135.3 (5)	C85—N12—Co8	108.7 (3)
Co6—O18—Co7	100.68 (19)	Co8—N12—H12B	109.9
C75—O19—Co9	108.9 (3)	Co8—N12—H12C	109.9
C75—O19—Co3	108.7 (3)	Co3—O19—Co4	91.14 (14)
Co9—O19—Co3	134.78 (19)	C84—O20—Co8	110.6 (3)
C75—O19—Co4	133.9 (4)	C84—O20—Co10	131.1 (4)
Co9—O19—Co4	80.26 (13)	Co8—O20—Co10	99.81 (18)

***R*-1**			
Co1—O8	1.982 (8)	Co6—O12	1.927 (9)
Co1—O22	2.056 (6)	Co6—O14	1.966 (7)
Co1—O21	2.123 (7)	Co6—N10	1.971 (10)
Co1—O5	2.194 (7)	Co7—O18	1.992 (8)
Co1—O4	2.222 (7)	Co7—N2	2.036 (9)
Co1—O17	2.224 (8)	Co7—O6	2.081 (8)
Co1—Co5	2.757 (3)	Co7—O14	2.114 (8)
Co2—O22	2.052 (7)	Co7—O3	2.135 (9)
Co2—O13	2.055 (7)	Co7—O4	2.204 (7)
Co2—N7	2.064 (9)	Co8—N1	1.882 (11)
Co2—O12	2.161 (8)	Co8—O20	1.913 (8)
Co2—O14	2.170 (7)	Co8—O1	1.941 (9)
Co2—O17	2.198 (7)	Co8—N12	1.941 (9)
Co3—O21	2.050 (7)	Co8—O2	1.960 (8)
Co3—O8	2.055 (8)	Co8—O7	1.978 (7)
Co3—N4	2.075 (9)	Co9—N8	1.843 (9)
Co3—O2	2.148 (7)	Co9—O16	1.915 (8)
Co3—O7	2.170 (8)	Co9—O15	1.931 (8)
Co3—O19	2.208 (7)	Co9—O19	1.943 (7)
Co4—O13	2.026 (7)	Co9—N11	1.948 (9)
Co4—O21	2.065 (6)	Co9—O9	1.954 (7)
Co4—O15	2.111 (7)	Co10—N5	1.987 (6)

Co4—O22	2.119 (7)	Co10—O20	2.040 (8)
Co4—O9	2.190 (7)	Co10—O7	2.094 (7)
Co4—O19	2.294 (7)	Co10—O16	2.101 (8)
Co4—Co9	2.740 (2)	Co10—O10	2.151 (8)
Co5—N3	1.871 (9)	Co10—O9	2.209 (7)
Co5—O6	1.895 (8)	Co5—O4	1.963 (7)
Co5—N9	1.910 (9)	Co6—N6	1.819 (6)
Co5—O5	1.910 (7)	Co6—O11	1.883 (8)
Co5—O17	1.948 (7)	Co6—O18	1.910 (7)
O8—Co1—O22	105.5 (3)	O21—Co3—O2	90.3 (3)
O8—Co1—O21	82.3 (3)	O8—Co3—O2	99.5 (3)
O22—Co1—O21	82.1 (2)	N4—Co3—O2	96.1 (3)
O8—Co1—O5	98.2 (3)	O21—Co3—O7	122.2 (3)
O22—Co1—O5	155.9 (3)	O8—Co3—O7	154.9 (3)
O21—Co1—O5	105.8 (3)	N4—Co3—O7	78.2 (4)
O8—Co1—O4	112.0 (3)	O2—Co3—O7	77.1 (3)
O22—Co1—O4	90.5 (3)	O21—Co3—O19	84.2 (3)
O21—Co1—O4	165.4 (3)	O8—Co3—O19	99.8 (3)
O5—Co1—O4	76.3 (2)	N4—Co3—O19	96.0 (3)
O8—Co1—O17	170.9 (3)	O2—Co3—O19	159.0 (3)
O22—Co1—O17	82.2 (3)	O7—Co3—O19	88.7 (3)
O21—Co1—O17	94.2 (3)	O13—Co4—O21	103.3 (3)
O5—Co1—O17	74.6 (3)	O13—Co4—O15	99.2 (3)
O4—Co1—O17	72.2 (3)	O21—Co4—O15	156.7 (3)
O8—Co1—Co5	132.7 (2)	O13—Co4—O22	82.5 (3)
O22—Co1—Co5	113.6 (2)	O21—Co4—O22	82.0 (2)
O21—Co1—Co5	127.5 (2)	O15—Co4—O22	107.2 (3)
O5—Co1—Co5	43.57 (19)	O13—Co4—O9	111.3 (3)
O4—Co1—Co5	44.86 (19)	O21—Co4—O9	88.1 (3)
O17—Co1—Co5	44.47 (17)	O15—Co4—O9	78.0 (3)
O22—Co2—O13	83.5 (3)	O22—Co4—O9	164.6 (3)
O22—Co2—N7	161.7 (4)	O13—Co4—O19	174.6 (3)
O13—Co2—N7	78.9 (4)	O21—Co4—O19	81.7 (3)
O22—Co2—O12	90.3 (3)	O15—Co4—O19	76.1 (3)
O13—Co2—O12	101.5 (3)	O22—Co4—O19	96.3 (3)
N7—Co2—O12	98.1 (3)	O9—Co4—O19	70.6 (3)
O22—Co2—O14	122.0 (3)	O13—Co4—Co9	133.3 (2)

O13—Co2—O14	154.1 (3)	O21—Co4—Co9	113.0 (2)
N7—Co2—O14	76.0 (4)	O15—Co4—Co9	44.6 (2)
O12—Co2—O14	76.1 (3)	O22—Co4—Co9	129.5 (2)
O22—Co2—O17	83.0 (3)	O9—Co4—Co9	45.02 (19)
O13—Co2—O17	99.4 (3)	O19—Co4—Co9	44.33 (17)
N7—Co2—O17	94.9 (3)	N3—Co5—O6	85.9 (4)
O12—Co2—O17	157.2 (3)	N3—Co5—N9	95.8 (4)
O14—Co2—O17	89.0 (3)	O6—Co5—N9	93.3 (4)
O21—Co3—O8	82.4 (3)	N3—Co5—O5	86.1 (4)
O21—Co3—N4	159.6 (4)	O6—Co5—O5	171.2 (3)
O8—Co3—N4	77.5 (4)	N9—Co5—O5	91.2 (4)
O18—Co7—O6	162.9 (3)	N3—Co5—O17	173.8 (4)
N2—Co7—O6	97.0 (3)	O6—Co5—O17	100.0 (3)
O18—Co7—O14	75.0 (3)	N9—Co5—O17	85.9 (3)
N2—Co7—O14	171.4 (3)	O5—Co5—O17	87.8 (3)
O6—Co7—O14	89.9 (3)	N3—Co5—O4	94.3 (4)
O18—Co7—O3	96.8 (3)	O6—Co5—O4	87.2 (3)
N2—Co7—O3	79.6 (4)	N9—Co5—O4	169.9 (3)
O6—Co7—O3	92.6 (3)	O5—Co5—O4	89.6 (3)
O14—Co7—O3	95.1 (3)	O17—Co5—O4	84.1 (3)
O18—Co7—O4	100.3 (3)	N3—Co5—Co1	121.3 (3)
N2—Co7—O4	77.3 (3)	O6—Co5—Co1	130.2 (2)
O6—Co7—O4	76.8 (3)	N9—Co5—Co1	120.7 (3)
O14—Co7—O4	109.4 (3)	O5—Co5—Co1	52.3 (2)
O3—Co7—O4	153.0 (3)	O17—Co5—Co1	53.1 (2)
N1—Co8—O20	177.2 (4)	O4—Co5—Co1	53.0 (2)
N1—Co8—O1	83.1 (4)	N6—Co6—O11	84.1 (4)
O20—Co8—O1	96.7 (4)	N6—Co6—O18	179.0 (4)
N1—Co8—N12	94.8 (4)	O11—Co6—O18	96.7 (4)
O20—Co8—N12	88.0 (4)	N6—Co6—O12	84.8 (4)
O1—Co8—N12	89.0 (4)	O11—Co6—O12	168.3 (4)
N1—Co8—O2	84.8 (4)	O18—Co6—O12	94.3 (4)
O20—Co8—O2	95.2 (3)	N6—Co6—O14	98.9 (3)
O1—Co8—O2	167.7 (4)	O11—Co6—O14	91.2 (3)
N12—Co8—O2	94.8 (4)	O18—Co6—O14	80.4 (3)
N1—Co8—O7	97.0 (4)	O12—Co6—O14	86.6 (3)
O20—Co8—O7	80.2 (3)	N6—Co6—N10	95.5 (4)

O1—Co8—O7	92.5 (3)	O11—Co6—N10	90.7 (4)
N12—Co8—O7	168.2 (3)	O18—Co6—N10	85.1 (4)
O2—Co8—O7	86.2 (3)	O12—Co6—N10	94.2 (4)
N8—Co9—O16	85.4 (4)	O14—Co6—N10	165.6 (4)
N8—Co9—O15	87.0 (4)	O18—Co7—N2	98.8 (3)
O16—Co9—O15	171.7 (3)	Co8—O2—Co3	98.1 (3)
N8—Co9—O19	176.0 (5)	C8—O3—Co7	112.3 (9)
O16—Co9—O19	98.5 (3)	C14—O4—Co5	125.6 (6)
O15—Co9—O19	89.1 (3)	C14—O4—Co7	108.7 (6)
N8—Co9—N11	94.4 (4)	Co5—O4—Co7	93.1 (3)
O16—Co9—N11	94.4 (4)	C14—O4—Co1	112.1 (6)
O15—Co9—N11	89.6 (4)	Co5—O4—Co1	82.2 (3)
O19—Co9—N11	86.3 (3)	Co7—O4—Co1	132.8 (3)
N8—Co9—O9	95.8 (3)	C15—O5—Co5	112.5 (6)
O16—Co9—O9	89.0 (3)	C15—O5—Co1	128.0 (7)
O15—Co9—O9	88.3 (3)	Co5—O5—Co1	84.1 (3)
O19—Co9—O9	83.4 (3)	C21—O6—Co5	110.7 (6)
N11—Co9—O9	169.5 (3)	C21—O6—Co7	118.6 (7)
N8—Co9—Co4	121.0 (4)	Co5—O6—Co7	99.1 (4)
O16—Co9—Co4	132.4 (2)	C22—O7—Co8	121.5 (7)
O15—Co9—Co4	50.2 (2)	C22—O7—Co10	121.4 (7)
O19—Co9—Co4	55.6 (2)	Co8—O7—Co10	96.6 (3)
N11—Co9—Co4	119.3 (3)	C22—O7—Co3	111.2 (7)
O9—Co9—Co4	52.4 (2)	Co8—O7—Co3	96.8 (3)
N5—Co10—O20	96.5 (3)	Co10—O7—Co3	105.7 (3)
N5—Co10—O7	167.8 (3)	C28—O8—Co1	142.4 (7)
O20—Co10—O7	74.7 (3)	C28—O8—Co3	117.2 (7)
N5—Co10—O16	97.0 (3)	Co1—O8—Co3	99.8 (3)
O20—Co10—O16	164.5 (3)	C29—O9—Co9	124.6 (7)
O7—Co10—O16	92.9 (3)	C29—O9—Co4	110.1 (6)
N5—Co10—O10	78.9 (4)	Co9—O9—Co4	82.6 (3)
O20—Co10—O10	96.6 (3)	C29—O9—Co10	108.7 (6)
O7—Co10—O10	93.6 (3)	Co9—O9—Co10	92.5 (3)
O16—Co10—O10	93.4 (3)	Co4—O9—Co10	135.7 (3)
N5—Co10—O9	80.1 (3)	C35—O10—Co10	111.5 (8)
O20—Co10—O9	97.0 (3)	C36—O11—Co6	116.2 (9)
O7—Co10—O9	109.0 (3)	C36—O11—H11B	121.9

O16—Co10—O9	78.0 (3)	Co6—O11—H11B	121.9
O10—Co10—O9	156.0 (3)	C42—O12—Co6	110.3 (7)
C1—O1—Co8	113.7 (8)	C42—O12—Co2	115.3 (8)
C1—O1—H1C	123.2	C75—O19—Co4	132.4 (6)
Co8—O1—H1C	123.2	Co9—O19—Co4	80.1 (2)
C7—O2—Co8	112.5 (6)	Co3—O19—Co4	91.2 (3)
C7—O2—Co3	115.8 (7)	C84—O20—Co8	108.6 (6)
Co6—O12—Co2	98.8 (4)	C84—O20—Co10	132.2 (7)
C43—O13—Co4	142.4 (7)	Co8—O20—Co10	100.6 (4)
C43—O13—Co2	118.8 (6)	Co3—O21—Co4	102.9 (3)
Co4—O13—Co2	98.4 (3)	Co3—O21—Co1	95.4 (3)
C49—O14—Co6	121.6 (6)	Co4—O21—Co1	97.7 (3)
C49—O14—Co7	121.2 (6)	Co3—O21—H4B	118.8
Co6—O14—Co7	95.3 (3)	Co4—O21—H4B	118.8
C49—O14—Co2	111.7 (6)	Co1—O21—H4B	118.8
Co6—O14—Co2	97.2 (3)	C93—O22—Co2	118.33 (19)
Co7—O14—Co2	106.2 (3)	C93—O22—Co1	119.3 (2)
C50—O15—Co9	110.5 (6)	Co2—O22—Co1	102.2 (3)
C50—O15—Co4	126.5 (6)	C93—O22—Co4	119.0 (2)
Co9—O15—Co4	85.2 (3)	Co2—O22—Co4	95.6 (3)
C56—O16—Co9	110.4 (7)	Co1—O22—Co4	98.1 (3)
C56—O16—Co10	121.1 (7)	C93—O22—H22C	0.5
Co9—O16—Co10	97.1 (3)	Co2—O22—H22C	118.8
C57—O17—Co5	108.6 (6)	Co1—O22—H22C	118.9
C57—O17—Co2	113.9 (5)	Co4—O22—H22C	118.8
Co5—O17—Co2	134.3 (4)	O22—C93—H22C	0.6
C57—O17—Co1	116.9 (6)	O22—C93—H93A	109.5
Co5—O17—Co1	82.4 (3)	O22—C93—H93B	109.5
Co2—O17—Co1	92.6 (3)	H93A—C93—H93B	109.5
C66—O18—Co6	113.6 (7)	O22—C93—H93C	109.5
C66—O18—Co7	134.5 (9)	H93A—C93—H93C	109.5
Co6—O18—Co7	101.2 (4)	H93B—C93—H93C	109.5
C75—O19—Co9	111.4 (6)	C6—N1—C2	126.9 (13)
C75—O19—Co3	107.4 (5)	C6—N1—Co8	115.4 (9)
Co9—O19—Co3	134.4 (4)	C2—N1—Co8	117.7 (11)
C9—N2—Co7	116.8 (9)	C13—N2—C9	120.7 (11)
C20—N3—Co5	118.9 (9)	C27—N4—Co3	117.7 (9)

C16—N3—Co5	118.0 (9)	C23—N4—Co3	118.8 (9)
C44—N7—C48	122.0 (11)	Co5—N9—H12B	109.4
C44—N7—Co2	116.2 (9)	C58—N9—H12C	109.4
C48—N7—Co2	121.1 (8)	Co5—N9—H12C	109.4
C51—N8—Co9	116.3 (10)	C67—N10—Co6	103.7 (7)
C55—N8—Co9	115.9 (9)	Co6—N10—H8C	111.0
C58—N9—Co5	111.1 (7)	Co6—N10—H8D	111.0
Co9—N11—H3C	110.1	C76—N11—Co9	108.0 (7)
C85—N12—Co8	108.6 (6)	Co9—N11—H3B	110.1
Co8—N12—H10B	110.0		

Table S3 Bond valence sum calculations for ***S*-1** and ***R*-1** based on the program BVS. *d* is the bond distances around metal center in angstrom unit.

***S*-1**			***R*-1**		
Co1	**1.970**		**Co1**	**1.917**	
Co1-O8	0.467	d=1.974(4)	Co1-O8	0.479	d=1.964(8)
Co1-O22	0.390	d=2.040(3)	Co1-O22	0.385	d=2.045(6)
Co1-O21	0.313	d=2.122(4)	Co1-O21	0.307	d=2.129(7)
Co1-O5	0.275	d=2.170(3)	Co1-O5	0.266	d=2.182(7)
Co1-O4	0.265	d=2.183(4)	Co1-O4	0.246	d=2.211(8)
Co1-O17	0.260	d=2.190(3)	Co1-O17	0.234	d=2.230(8)
Co2	**2.162**		**Co2**	**2.082**	
Co2-N7	0.564	d=2.052(4)	Co2-O22	0.336	d=2.095(7)
Co2-O13	0.385	d=2.045(4)	Co2-O13	0.386	d=2.044(7)
Co2-O22	0.369	d=2.061(3)	Co2-N7	0.549	d=2.062(9)
Co2-O12	0.306	d=2.130(3)	Co2-O12	0.278	d=2.165(8)
Co2-O14	0.286	d=2.155(4)	Co2-O14	0.269	d=2.178(7)
Co2-O17	0.252	d=2.202(3)	Co2-O17	0.263	d=2.186(7)
Co3	**2.150**		**Co3**	**2.039**	
Co3-O8	0.390	d=2.040(4)	Co3-O21	0.379	d=2.051(7)

Co3-N4	0.565	d=2.051(4)	Co3-O8	0.350	d=2.080(8)
Co3-O21	0.377	d=2.053(3)	Co3-N4	0.509	d=2.090(9)
Co3-O2	0.282	d=2.160(3)	Co3-O2	0.284	d=2.158(8)
Co3-O7	0.276	d=2.168(4)	Co3-O7	0.279	d=2.164(8)
Co3-O19	0.259	d=2.192(3)	Co3-O19	0.237	d=2.224(7)
Co4	**1.954**		**Co4**	**1.859**	
Co4-O13	0.421	d=2.012(4)	Co4-O13	0.386	d=2.044(7)
Co4-O21	0.398	d=2.033(3)	Co4-O21	0.380	d=2.050(6)
Co4-O15	0.352	d=2.078(4)	Co4-O15	0.329	d=2.103(7)
Co4-O22	0.334	d=2.098(3)	Co4-O22	0.314	d=2.121(7)
Co4-O	9 0.246	d=2.211(4)	Co4-O9	0.253	d=2.201(7)
Co4-O19	0.203	d=2.282(4)	Co4-O19	0.197	d=2.293(8)
Co5	**4.009**		**Co5**	**3.873**	
Co5-N3	1.061	d=1.818(4)	Co5-N3	0.981	d=1.847(10)
Co5-O5	0.578	d=1.895(4)	Co5-O6	0.558	d=1.908(8)
Co5-O6	0.552	d=1.912(4)	Co5-N9	0.817	d=1.915(9)
Co5-N9	0.803	d=1.921(5)	Co5-O5	0.537	d=1.922(7)
Co5-O17	0.521	d=1.933(3)	Co5-O17	0.497	d=1.951(7)
Co5-O4	0.494	d=1.953(4)	Co5-O4	0.483	d=1.961(8)
Co6	**3.902**		**Co6**	**3.912**	
Co6-N6	0.973	d=1.850(5)	Co6-N6	1.039	d=1.826(6)
Co6-O18	0.586	d=1.890(4)	Co6-O11	0.635	d=1.860(9)
Co6-O11	0.573	d=1.898(4)	Co6-O18	0.565	d=1.903(7)
Co6-O12	0.523	d=1.932(4)	Co6-O12	0.536	d=1.923(9)
Co6-N10	0.757	d=1.943(5)	Co6-O14	0.483	d=1.961(7)
Co6-O14	0.490	d=1.956(3)	Co6-N10	0.654	d=1.997(10)
Co7	**2.270**		**Co7**	**2.153**	
Co7-O18	0.430	d=2.004(4)	Co7-O18	0.428	d=2.006(8)
Co7-N2	0.621	d=2.016(5)	Co7-N2	0.531	d=2.074(9)

Co7-O6	0.358	d=2.072(4)	Co7-O6	0.350	d=2.080(8)
Co7-O14	0.332	d=2.100(4)	Co7-O14	0.311	d=2.124(8)
Co7-O3	0.289	d=2.151(4)	Co7-O3	0.295	d=2.144(9)
Co7-O4	0.239	d=2.222(4)	Co7-O4	0.237	d=2.224(7)
Co8	**4.009**		**Co8**	**3.754**	
Co8-N1	1.022	d=1.832(5)	Co8-N1	0.912	d=1.874(11)
Co8-O20	0.587	d=1.889(4)	Co8-O20	0.573	d=1.898(8)
Co8-O1	0.578	d=1.895(4)	Co8-O1	0.521	d=1.933(9)
Co8-N12	0.803	d=1.921(5)	Co8-N12	0.778	d=1.933(10)
Co8-O2	0.528	d=1.928(4)	Co8-O2	0.490	d=1.956(9)
Co8-O7	0.490	d=1.956(3)	Co8-O7	0.479	d=1.964(7)
Co9	**3.993**		**Co9**	**3.809**	
Co9-N8	1.061	d=1.818(4)	Co9-N8	1.008	d=1.837(10)
Co9-O15	0.575	d=1.897(4)	Co9-O16	0.546	d=1.916(8)
Co9-O16	0.562	d=1.905(4)	Co9-O15	0.547	d=1.915(8)
Co9-O19	0.536	d=1.923(3)	Co9-O19	0.524	d=1.931(7)
Co9-N11	0.753	d=1.945(4)	Co9-N11	0.692	d=1.976(10)
Co9-O9	0.506	d=1.944(3)	Co9-O9	0.491	d=1.955(8)
Co10	**2.265**		**Co10**	**2.280**	
Co10-N5	0.649	d=2.000(5)	Co10-N5	0.694	d=1.975(6)
Co10-O20	0.372	d=2.058(4)	Co10-O20	0.377	d=2.053(8)
Co10-O7	0.347	d=2.084(4)	Co10-O7	0.334	d=2.098(7)
Co10-O16	0.332	d=2.100(4)	Co10-O16	0.328	d=2.105(8)
Co10-O10	0.304	d=2.133(4)	Co10-O10	0.311	d=2.124(9)
Co10-O9	0.262	d=2.188(4)	Co10-O9	0.237	d=2.225(7)
O1	**0.578**		**O1**	**0.521**	
Co8-O1	0.578	d=1.895(4)	Co8-O1	0.521	d=1.933(9)
O3	**0.289**		**O3**	**0.295**	
Co7-O3	0.289	d=2.151(4)	Co7-O3	0.295	d=2.144(9)

O10	**0.304**		**O10**	**0.311**	
Co10-O10	0.304	d=2.133(4)	Co10-O10	0.311	d=2.124(9)
O11	**0.573**		**O11**	**0.635**	
Co6-O11	0.573	d=1.898(4)	Co6-O11	0.635	d=1.860(9)
O21	**1.088**		**O21**	**1.066**	
Co1-O21	0.313	d=2.122(4)	Co1-O21	0.307	d=2.129(7)
Co3-O21	0.377	d=2.053(3)	Co3-O21	0.379	d=2.051(7)
Co4-O21	0.398	d=2.033(3)	Co4-O21	0.380	d=2.050(6)
O22	**1.093**		**O22**	**1.035**	
Co1-O22	0.390	d=2.040(3)	Co1-O22	0.385	d=2.045(6)
Co2-O22	0.369	d=2.061(3)	Co2-O22	0.336	d=2.095(7)
Co4-O22	0.334	d=2.098(3)	Co4-O22	0.314	d=2.121(7)

Table S4 Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2) for ***S*-1** and ***R*-1**

***S*-1**

***S*-1**	x	y	z	U_{iso}*/U_{eq}	Occ. (<1)
O21	0.1927 (3)	0.71540 (15)	0.1566 (2)	0.0474 (8)	
H21C	0.1453	0.7423	0.1251	0.057*	
O22	0.3257 (3)	0.70337 (14)	0.3253 (2)	0.0460 (8)	
H22C	0.3732	0.6768	0.3579	0.055*	**0.50**
C93	0.4006 (7)	0.6641 (4)	0.3658 (7)	0.044 (2)	**0.50**
H93A	0.4608	0.6819	0.3896	0.066*	**0.50**
H93B	0.4032	0.6390	0.3174	0.066*	**0.50**
H93C	0.3867	0.6455	0.4170	0.066*	**0.50**
Cl1	0.1594 (3)	0.46696 (10)	0.52080 (17)	0.1260 (11)	
O23	0.2218 (8)	0.4438 (5)	0.5996 (7)	0.159 (5)	0.665 (17)

O24	0.0712 (6)	0.4735 (7)	0.5363 (10)	0.178 (5)	0.665 (17)
O25	0.1479 (12)	0.4359 (5)	0.4413 (7)	0.207 (6)	0.665 (17)
O26	0.1922 (11)	0.5170 (3)	0.5065 (7)	0.149 (5)	0.665 (17)
O23B	0.1383 (18)	0.4515 (9)	0.4268 (7)	0.155 (6)	0.335 (17)
O24B	0.2449 (11)	0.4948 (10)	0.5473 (19)	0.167 (8)	0.335 (17)
O25B	0.0883 (13)	0.4992 (8)	0.5323 (18)	0.172 (8)	0.335 (17)
O26B	0.170 (2)	0.4226 (6)	0.5784 (15)	0.179 (8)	0.335 (17)
Cl2	0.5541 (2)	0.71184 (9)	0.91979 (16)	0.1054 (8)	
O27	0.5955 (15)	0.6686 (6)	0.8915 (12)	0.158 (7)	0.395 (11)
O28	0.5718 (12)	0.7571 (5)	0.8746 (9)	0.105 (5)	0.395 (11)
O29	0.4553 (6)	0.7046 (9)	0.8916 (13)	0.180 (7)	0.395 (11)
O30	0.5867 (14)	0.7183 (7)	1.0166 (5)	0.144 (8)	0.395 (11)
O27B	0.5145 (10)	0.6625 (3)	0.8933 (9)	0.153 (5)	0.605 (11)
O28B	0.6425 (6)	0.7128 (6)	0.9019 (9)	0.160 (5)	0.605 (11)
O29B	0.4983 (11)	0.7519 (5)	0.8710 (8)	0.191 (6)	0.605 (11)
O30B	0.5709 (8)	0.7186 (5)	1.0167 (4)	0.110 (4)	0.605 (11)
Cl3	0.35505 (17)	0.95798 (7)	0.97474 (13)	0.0853 (6)	
O31	0.4388 (5)	0.9480 (4)	0.9501 (6)	0.135 (4)	0.759 (9)
O32	0.2938 (6)	0.9864 (3)	0.9043 (6)	0.138 (4)	0.759 (9)
O33	0.3177 (6)	0.9087 (2)	0.9859 (5)	0.104 (3)	0.759 (9)
O34	0.3804 (7)	0.9848 (3)	1.0605 (5)	0.121 (3)	0.759 (9)
O31B	0.370 (2)	0.9846 (10)	0.8997 (13)	0.151 (8)	0.241 (9)
O32B	0.2650 (9)	0.9715 (10)	0.9813 (19)	0.130 (7)	0.241 (9)
O33B	0.3577 (18)	0.9038 (3)	0.963 (2)	0.125 (8)	0.241 (9)
O34B	0.4224 (14)	0.9725 (11)	1.0591 (11)	0.136 (8)	0.241 (9)
Cl4	−0.0448 (4)	0.7174 (2)	0.5635 (3)	0.1106 (19)	0.539 (6)

O35	−0.0715 (10)	0.7070 (6)	0.4675 (5)	0.136 (6)	0.539 (6)
O36	0.0394 (8)	0.6921 (6)	0.6097 (9)	0.196 (9)	0.539 (6)
O37	−0.1147 (9)	0.6997 (7)	0.6017 (10)	0.193 (8)	0.539 (6)
O38	−0.0334 (12)	0.7716 (3)	0.5788 (11)	0.192 (8)	0.539 (6)
O4W	0.0668 (19)	0.8054 (13)	0.738 (2)	0.140 (8)	**0.270 (3)**
Cl4B	−0.1378 (5)	0.6803 (3)	0.5261 (4)	0.124 (3)	0.461 (6)
O35B	−0.1548 (13)	0.7213 (6)	0.5820 (10)	0.173 (9)	0.461 (6)
O36B	−0.2163 (9)	0.6748 (6)	0.4464 (8)	0.172 (8)	0.461 (6)
O37B	−0.0590 (10)	0.6935 (8)	0.4979 (13)	0.196 (10)	0.461 (6)
O38B	−0.1210 (14)	0.6336 (5)	0.5761 (11)	0.228 (11)	0.461 (6)
O5W	0.0499 (15)	0.7582 (11)	0.6667 (16)	0.087 (7)	**0.230 (3)**
O1W	0.1724 (4)	0.8029 (2)	0.9859 (4)	0.0842 (14)	
O2W	0.1255 (6)	0.8882 (3)	0.8655 (7)	0.151 (3)	
O3W	0.3742 (15)	0.6214 (7)	0.5372 (17)	0.192 (9)	**0.50**
O6W	0.0158 (12)	0.8706 (7)	0.6740 (10)	0.133 (5)	**0.50**

***R*-1**

	x	y	z	U_{iso}*/U_{eq}	Occ. (<1)
O21	0.8441 (4)	0.1279 (3)	0.3061 (5)	0.052 (2)	
H4B	0.8756	0.1542	0.3516	0.063*	
O22	0.6732 (4)	0.1169 (3)	0.1757 (5)	0.053 (2)	
H22C	0.6446	0.0946	0.1359	0.063*	**0.50**
C93	0.6199 (4)	0.0763 (3)	0.1024 (5)	0.29 (3)	**0.50**
H93A	0.6496	0.0730	0.0554	0.441*	**0.50**
H93B	0.5569	0.0876	0.0750	0.441*	**0.50**
H93C	0.6203	0.0433	0.1319	0.441*	**0.50**

Cl1	0.0255 (3)	0.37067 (15)	0.1470 (3)	0.0968 (12)	
O23	0.0163 (8)	0.3209 (3)	0.1884 (9)	0.109 (4)	0.694 (9)
O24	0.0965 (7)	0.4000 (4)	0.2101 (8)	0.124 (4)	0.694 (9)
O25	0.0495 (8)	0.3607 (5)	0.0636 (6)	0.127 (4)	0.694 (9)
O26	−0.0625 (6)	0.3971 (5)	0.1232 (8)	0.116 (4)	0.694 (9)
O23B	0.0221 (18)	0.3149 (3)	0.1383 (18)	0.116 (5)	0.306 (9)
O24B	0.0219 (18)	0.3840 (10)	0.2386 (8)	0.116 (5)	0.306 (9)
O25B	0.1097 (10)	0.3899 (9)	0.1359 (19)	0.124 (5)	0.306 (9)
O26B	−0.0535 (12)	0.3930 (9)	0.0791 (13)	0.123 (5)	0.306 (9)
Cl2	0.5197 (3)	0.37828 (19)	0.6577 (4)	0.150 (2)	
O27	0.4414 (9)	0.3456 (6)	0.6509 (15)	0.202 (7)	0.669 (19)
O28	0.6018 (8)	0.3573 (8)	0.7233 (11)	0.183 (7)	0.669 (19)
O29	0.5341 (13)	0.3824 (9)	0.5687 (7)	0.195 (7)	0.669 (19)
O30	0.5038 (11)	0.4294 (4)	0.6885 (15)	0.164 (6)	0.669 (19)
O27B	0.4222 (8)	0.3656 (13)	0.628 (2)	0.178 (8)	0.331 (19)
O28B	0.543 (2)	0.4053 (15)	0.7448 (16)	0.195 (9)	0.331 (19)
O29B	0.573 (2)	0.3312 (8)	0.669 (3)	0.185 (8)	0.331 (19)
O30B	0.540 (2)	0.4107 (12)	0.590 (2)	0.183 (9)	0.331 (19)
Cl3	0.9128 (10)	0.6263 (6)	0.0465 (10)	0.146 (5)	0.459 (12)
O31	0.8659 (15)	0.6589 (10)	0.0950 (15)	0.145 (7)	0.459 (12)
O32	0.8741 (17)	0.6350 (10)	−0.0511 (10)	0.156 (7)	0.459 (12)
O33	1.0100 (10)	0.6385 (11)	0.0766 (19)	0.138 (7)	0.459 (12)
O34	0.9002 (17)	0.5726 (7)	0.0670 (19)	0.163 (7)	0.459 (12)
Cl3B	0.9235 (7)	0.6233 (4)	0.0593 (8)	0.105 (3)	0.541 (12)
O31B	0.9069 (13)	0.6136 (8)	0.1469 (8)	0.142 (6)	0.541 (12)
O32B	0.8805 (13)	0.6717 (6)	0.0230 (16)	0.154 (7)	0.541 (12)

O33B	1.0212 (8)	0.6255 (9)	0.0743 (16)	0.140 (7)	0.541 (12)
O34B	0.8829 (15)	0.5817 (7)	−0.0032 (13)	0.166 (7)	0.541 (12)
Cl4	0.4375 (6)	0.1303 (4)	0.5430 (7)	0.148 (4)	0.535 (5)
O35	0.3947 (12)	0.1013 (8)	0.4607 (11)	0.183 (7)	0.535 (5)
O36	0.4212 (13)	0.1849 (5)	0.5254 (14)	0.179 (7)	0.535 (5)
O37	0.5359 (7)	0.1208 (8)	0.5747 (13)	0.167 (7)	0.535 (5)
O38	0.3982 (13)	0.1148 (8)	0.6142 (11)	0.171 (7)	0.535 (5)
O4W	0.3246 (12)	0.2832 (8)	0.4828 (12)	0.127 (7)	**0.535 (5)**
Cl4B	0.4764 (6)	0.0917 (4)	0.6427 (6)	0.121 (3)	0.465 (5)
O35B	0.4256 (12)	0.0441 (5)	0.6238 (15)	0.178 (7)	0.465 (5)
O36B	0.4189 (12)	0.1327 (6)	0.6595 (15)	0.161 (7)	0.465 (5)
O37B	0.5561 (10)	0.0854 (8)	0.7238 (10)	0.161 (7)	0.465 (5)
O38B	0.5072 (14)	0.1058 (9)	0.5655 (11)	0.180 (8)	0.465 (5)
O5W	0.3256 (17)	0.1753 (13)	0.4459 (12)	0.194 (16)	**0.465 (5)**
O1W	0.0140 (6)	0.2139 (4)	0.3290 (6)	0.082 (3)	
O2W	0.1314 (7)	0.2994 (4)	0.3750 (7)	0.145 (4)	
O3W	0.4793 (14)	0.0373 (7)	0.1351 (15)	0.110 (7)	**0.50**

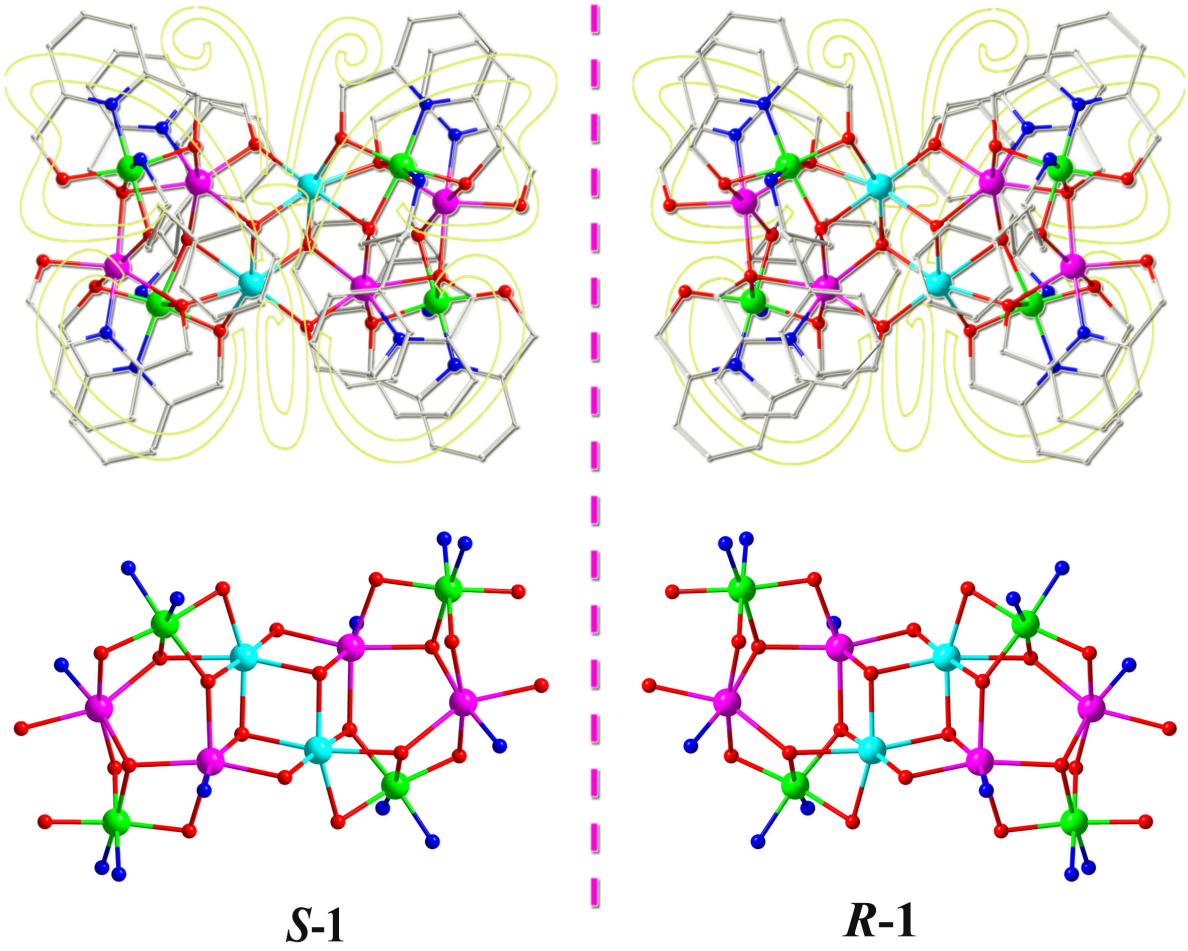


Fig. S4 The butterfly-like structures and [$Co^{II}_6Co^{III}_4$] core structures of ***S*-1** (left) and ***R*-1**(right).

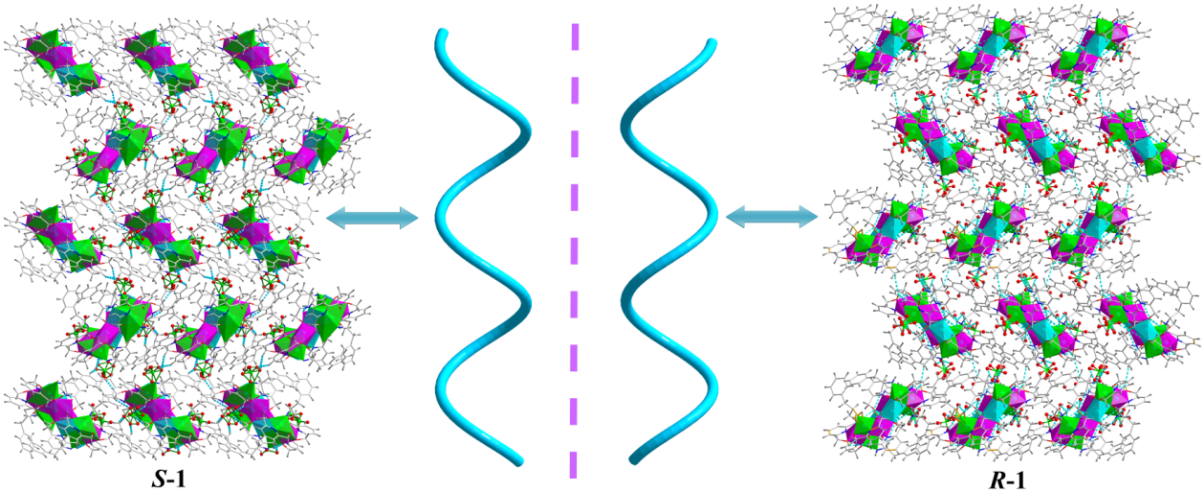


Fig. S5 The 3D supramolecular cluster complexes with left-handed (***S*-1**) and right-handed (***R*-1**) helices constructed by hydrogen bonding interactions.

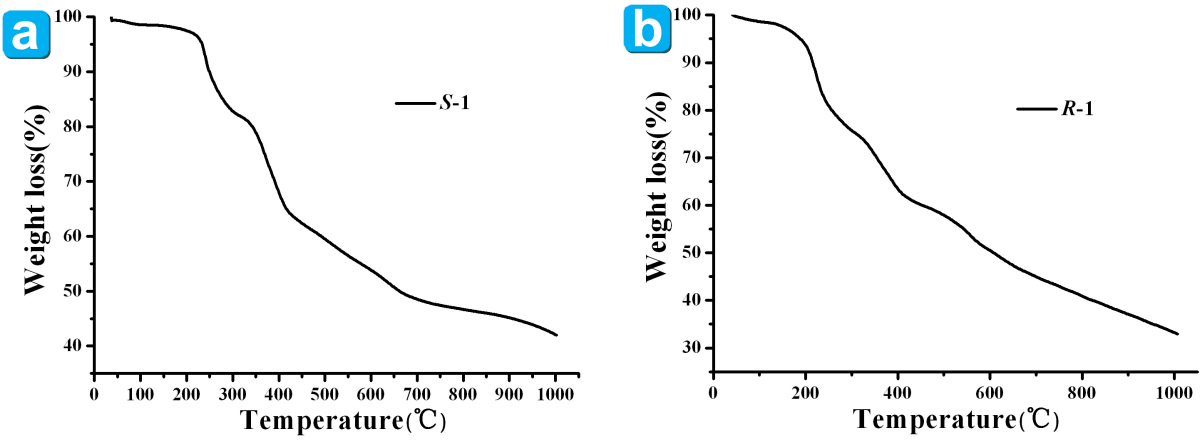


Fig. S6 TGA curves of ***S*-1** (a) and ***R*-1** (b).

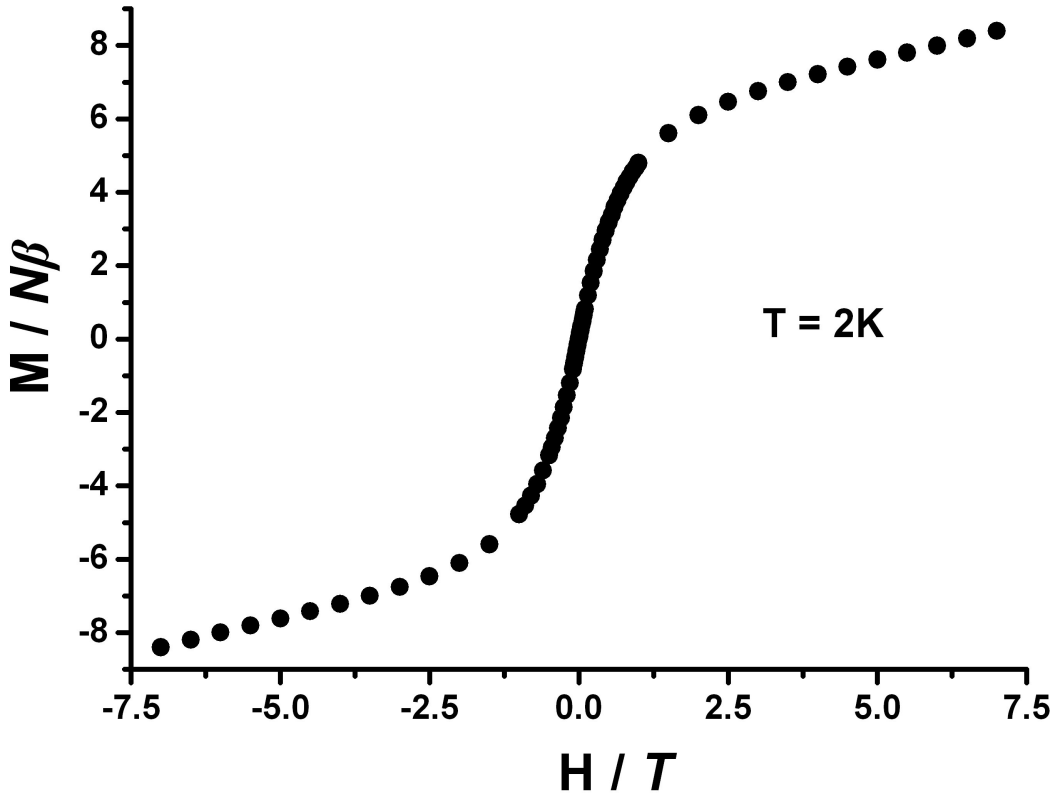


Fig. S7 Magnetization *M vs*. the magnetic field *H* for ***S*-1** at 2 K

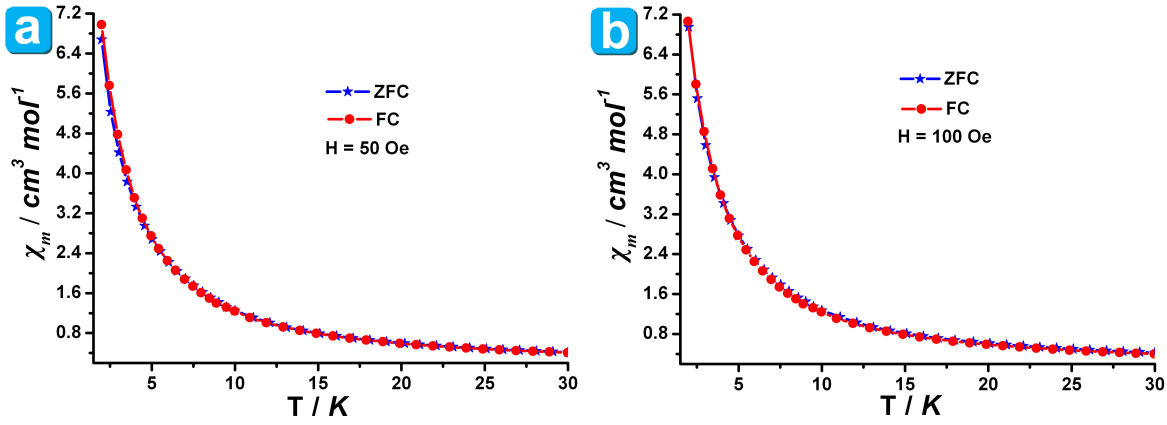


Fig. S8 The FC/ZFC curves at 2-30 K for ***S*-1** at 50 Oe (a) and 100 Oe (b).

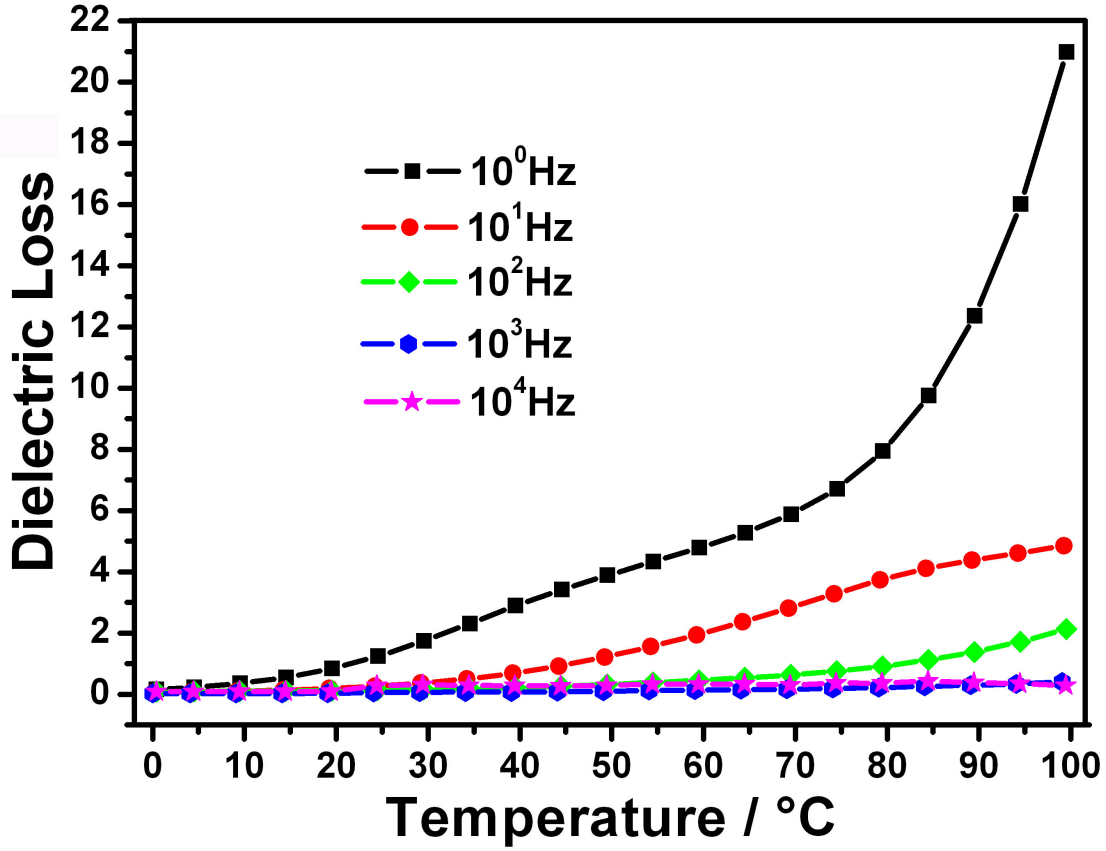


Fig. S9 The temperature dependence of the dielectric loss of ***S*-1** at various frequencies between 1 and 10^4 Hz.

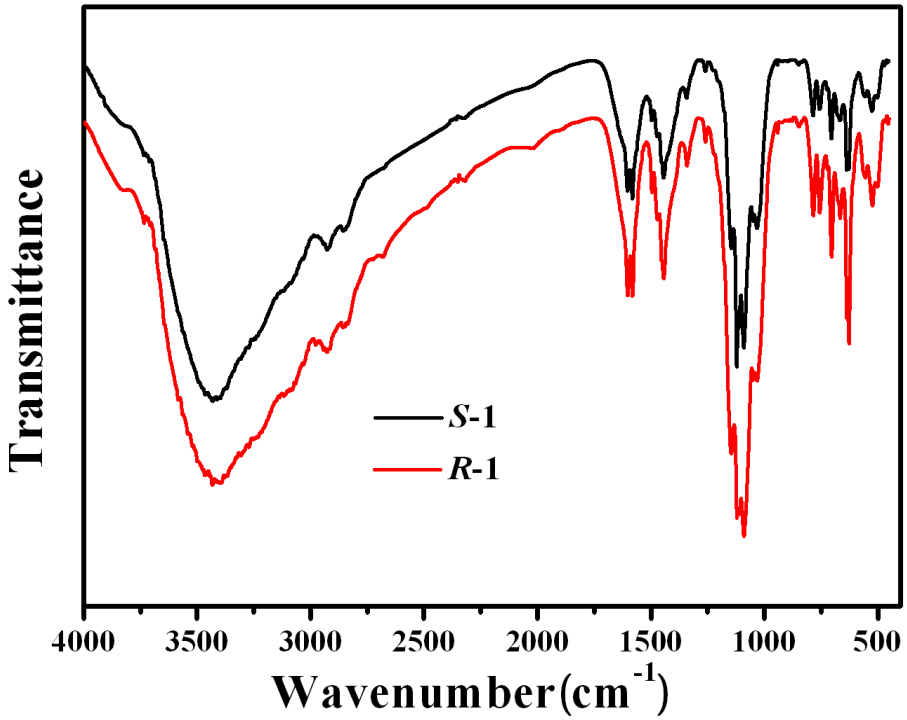


Fig. S10 IR spectra of ***S*-1** (black) and ***R*-1** (red).