Supplementary Material (ESI) for Dalton Transactions

A series of chiral coordination polymers containing helicals assembled from a new chiral (R)-2-(4'-(4''-carboxybenzyloxy)-phenoxy)-propanoic acid: syntheses, structures and photoluminescent properties

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Table 514 Selected bold distances (77) and angles (7) for 1.					
Ni(1)-O(6)	2.005(3)	Ni(1)-O(1W)	2.022(2)		
Ni(1)-O(2W)	2.023(3)	Ni(1)-O(1) ^{#1}	2.051(3)		
Ni(1)-O(4)	2.120(2)	Ni(1)-O(2) ^{#1}	2.177(3)		
O(6)-Ni(1)-O(1W)	93.95(11)	O(6)-Ni(1)-O(2W)	94.37(13)		
O(1W)-Ni(1)-O(2W)	92.33(12)	O(6)-Ni(1)-O(1) ^{#1}	159.86(11)		
O(1W)-Ni(1)-O(1) ^{#1}	98.56(11)	O(2W)-Ni(1)-O(1) ^{#1}	100.79(13)		
O(6)-Ni(1)-O(4)	77.27(10)	O(1W)-Ni(1)-O(4)	171.18(12)		
O(2W)-Ni(1)-O(4)	89.30(14)	O(1) ^{#1} -Ni(1)-O(4)	89.64(10)		
O(6)-Ni(1)-O(2) ^{#1}	101.78(11)	O(1W)-Ni(1)-O(2) ^{#1}	92.34(11)		
O(2W)-Ni(1)-O(2) ^{#1}	162.82(11)	O(1) ^{#1} -Ni(1)-O(2) ^{#1}	62.16(12)		
O(4)-Ni(1)-O(2) ^{#1}	88.60(11)				
Tal	Table S1b Hydrogen bonds for 1 (Å and °).				

Table S1a Selected bond distances (Å) and angles (°) for 1.

Table S1b Hydrogen bonds for 1 (A and $^{\circ}$).						
D-H···A	d(D-H)	$d(H \cdots A)$	$d(D \cdots A)$	<(DHA)		
$O(1W)-H(1A)\cdots O(5)^{\#3}$	0.898(10)	1.874(17)	2.742(4)	162(4)		
$O(1W)-H(1B)\cdots O(5)^{#4}$	0.897(10)	1.885(15)	2.768(4)	167(5)		
$O(2W)-H(2A)\cdots O(6)^{\#4}$	0.895(10)	1.869(16)	2.745(4)	166(4)		

Symmetry transformations used to generate equivalent atoms:

^{#1} -x+2, y+1/2, -z+2; ^{#3} x+1, y, z; ^{#4} -x+1, y-1/2, -z+1.

Table S2a Selected bond distances (Å) and angles (°) for 2.

Co(1)-O(6) ^{#1}	2.023(2)	Co(1)-O(1W)	2.0366(17)	
Co(1)-O(2W)	2.039(2)	Co(1)-O(1)	2.0441(18)	
Co(1)-O(4) ^{#1}	2.2066(16)	Co(1)-O(2)	2.275(2)	
O(6) ^{#1} -Co(1)-O(1W)	95.94(8)	O(6) ^{#1} -Co(1)-O(2W)	97.16(9)	
O(1W)-Co(1)-O(2W)	92.66(8)	O(6) ^{#1} -Co(1)-O(1)	151.83(8)	
O(1W)-Co(1)-O(1)	102.36(8)	O(2W)-Co(1)-O(1)	103.12(10)	
O(6) ^{#1} -Co(1)-O(4) ^{#1}	74.77(7)	O(1W)-Co(1)-O(4) ^{#1}	170.66(9)	
O(2W)-Co(1)-O(4) ^{#1}	89.56(9)	O(1)-Co(1)-O(4) ^{#1}	85.95(7)	

$O(6)^{\#1}-Co(1)-O(2)$	98.50(8)	O(1W)-Co(O(1W)-Co(1)-O(2)		
O(2W)-Co(1)-O(2)	163.46(8)	O(1)-Co(1	O(1)-Co(1)-O(2)		
O(4) ^{#1} -Co(1)-O(2)	89.47(8)				
Table S2bHydrogen bonds for 2 (Å and °).					
D-H···A	d(D-H)	$d(H \cdots A)$	$d(D \cdots A)$	<(DHA)	
$O(1W)-H(1A)\cdots O(5)^{\#3}$	0.901(10)	1.866(11)	2.765(3)	176(3)	
$O(1W)-H(1B)\cdots O(5)^{#4}$	0.893(10)	1.838(12)	2.717(3)	168(3)	
2 μ					

^{#1} -x, y-1/2, -z; ^{#3} x+1, y-1, z+1; ^{#4} -x-1, y-1/2, -z.

Table S3a Selected bond distances (Å) and angles (°) for 3.

$Cd(1)-O(5)^{\#1}$	2.275(6)	Cd(1)-O(6) ^{#2}	2.297(5)
Cd(1)-O(6)	2.331(5)	Cd(1)-O(1W)	2.332(5)
$Cd(1)-O(1)^{\#3}$	2.397(7)	$Cd(1)-O(2)^{\#3}$	2.417(7)
Cd(1)-O(4)	2.480(5)		
O(5) ^{#1} -Cd(1)-O(6) ^{#2}	99.0(2)	O(5) ^{#1} -Cd(1)-O(6)	140.8(2)
O(6) ^{#2} -Cd(1)-O(6)	107.73(15)	O(5) ^{#1} -Cd(1)-O(1W)	78.7(3)
O(6) ^{#2} -Cd(1)-O(1W)	82.2(2)	O(6)-Cd(1)-O(1W)	77.2(3)
O(5) ^{#1} -Cd(1)-O(1) ^{#3}	78.7(2)	$O(6)^{#2}-Cd(1)-O(1)^{#3}$	87.4(2)
O(6)-Cd(1)-O(1) ^{#3}	129.6(2)	O(1W)-Cd(1)-O(1) ^{#3}	153.2(3)
$O(5)^{\#1}-Cd(1)-O(2)^{\#3}$	131.4(2)	$O(6)^{#2}-Cd(1)-O(2)^{#3}$	88.5(2)
O(6)-Cd(1)-O(2) ^{#3}	78.4(2)	O(1W)-Cd(1)-O(2) ^{#3}	149.7(3)
O(1) ^{#3} -Cd(1)-O(2) ^{#3}	53.6(2)	O(1) ^{#3} -Cd(1)-O(4)	93.7(2)
O(5) ^{#1} -Cd(1)-O(4)	85.47(19)	O(6) ^{#2} -Cd(1)-O(4)	175.51(18)
O(1W)-Cd(1)-O(4)	98.6(2)	O(6)-Cd(1)-O(4)	68.28(18)
O(2) ^{#3} -Cd(1)-O(4)	88.7(2)		

Symmetry transformations used to generate equivalent atoms:

^{#1} x, y-1, z; ^{#2} -x+1/2 ,y-1/2, -z; ^{#3} -x+1, y, -z+1.

Cd(1)-O(2)	2.254(3)	$Cd(1)-O(5)^{\#1}$	2.269(3)
$Cd(1)-O(6)^{#2}$	2.370(3)	Cd(1)-N(1)	2.385(4)
$Cd(1)-O(5)^{#2}$	2.406(3)	Cd(1)-N(2)	2.414(4)
O(2)-Cd(1)-O(5) ^{#1}	94.66(12)	O(2)-Cd(1)-O(6) ^{#2}	130.13(12)
$O(5)^{#1}$ -Cd(1)-O(6) ^{#2}	95.82(11)	O(2)-Cd(1)-N(1)	81.95(13)
O(5) ^{#1} -Cd(1)-N(1)	111.11(11)	O(6) ^{#2} -Cd(1)-N(1)	136.88(11)
O(2)-Cd(1)-O(5) ^{#2}	100.70(12)	O(5) ^{#1} -Cd(1)-O(5) ^{#2}	149.87(6)
$O(6)^{#2}-Cd(1)-O(5)^{#2}$	54.63(10)	N(1)-Cd(1)-O(5) ^{#2}	96.70(11)
O(2)-Cd(1)-N(2)	149.11(14)	O(5) ^{#1} -Cd(1)-N(2)	86.34(13)
$O(6)^{#2}-Cd(1)-N(2)$	80.24(11)	N(1)-Cd(1)-N(2)	69.06(13)
O(5) ^{#2} -Cd(1)-N(2)	93.27(12)		

Table S4a Selected bond distances (Å) and angles (°) for 4.

Symmetry transformations used to generate equivalent atoms: ${}^{\#1}x+1/2$, -y+1/2, -z+1; ${}^{\#2}x$, y+1, z.

Table S5a Selected bond distances (Å) and angles (°) for 5.

$Mn(1)-O(2)^{\#1}$	2.071(3)	Mn(1)-O(1)	2.103(4)
Mn(1)-O(11)	2.200(3)	Mn(1)-N(2)	2.278(4)
Mn(1)-N(1)	2.282(4)	Mn(1)-O(12)	2.399(4)
Mn(2)-O(5)	2.492(11)	$Mn(2)-O(8)^{\#2}$	2.045(4)
Mn(2)-O(6)	2.093(4)	Mn(2)-O(7)	2.105(4)
Mn(2)-N(4)	2.258(5)	Mn(2)-N(3)	2.305(4)
O(2) ^{#1} -Mn(1)-O(1)	101.75(15)	O(2) ^{#1} -Mn(1)-O(11)	142.34(14)
O(1)-Mn(1)-O(11)	90.99(15)	$O(2)^{\#1}-Mn(1)-N(2)$	87.90(16)
O(1)-Mn(1)-N(2)	165.61(16)	O(11)-Mn(1)-N(2)	87.64(16)
$O(2)^{\#1}-Mn(1)-N(1)$	117.78(14)	O(1)-Mn(1)-N(1)	93.55(16)
O(11)-Mn(1)-N(1)	96.28(14)	N(2)-Mn(1)-N(1)	72.38(16)
O(2) ^{#1} -Mn(1)-O(12)	86.71(14)	O(1)-Mn(1)-O(12)	99.59(15)
O(11)-Mn(1)-O(12)	56.06(13)	N(2)-Mn(1)-O(12)	91.52(15)
N(1)-Mn(1)-O(12)	149.22(15)	O(8) ^{#2} -Mn(2)-O(6)	130.80(17)

O(8) ^{#2} -Mn(2)-O(7)	99.80(16)	O(6)-Mn(2)-O(7)	89.86(15)
O(8) ^{#2} -Mn(2)-N(4)	89.58(17)	O(6)-Mn(2)-N(4)	93.82(16)
O(7)-Mn(2)-N(4)	163.98(17)	$O(8)^{#2}-Mn(2)-N(3)$	119.12(16)
O(6)-Mn(2)-N(3)	108.66(17)	O(7)-Mn(2)-N(3)	91.18(17)
N(4)-Mn(2)-N(3)	72.87(17)	O(8) ^{#2} -Mn(2)-O(5)	81.7(4)
O(6)-Mn(2)-O(5)	49.6(4)	O(7)-Mn(2)-O(5)	107.2(4)
N(4)-Mn(2)-O(5)	86.9(4)	N(3)-Mn(2)-O(5)	150.0(3)

Table S5b Hydrogen bonds for 5 (Å and °).

D-H···A	d(D-H)	$d(H \cdots A)$	$d(D \cdots A)$	<(DHA)
O(1W)-H(1A) ···O(10) ^{#4}	0.898(10)	2.34(6)	3.043(3)	135(7)
C(42)-H(42) ····O(1W)	0.93	2.60	3.385(9)	142.9
C(25)-H(25A) ····O(11) ^{#5}	0.97	2.27	3.041(7)	135.3
$C(52)-H(52)\cdots O(5)^{\#5}$	0.93	2.56	3.392(14)	149.5
C(54)-H(54) ····O(2W)	0.93	2.57	3.417(12)	151.5

^{#1} -x+1, y, -z+2; ^{#2} -x+1, y, -z+1; ^{#4} x, y-1, z; ^{#5} x, y+1, z.

 Table S6a Selected bond distances (Å) and angles (°) for 6.

Cd(1)-N(1)	2.196(8)	$Cd(1)-N(4)^{\#1}$	2.229(8)
Cd(1)-O(12)	2.263(6)	Cd(1)-O(2) ^{#2}	2.324(6)
Cd(1)-O(1) ^{#2}	2.421(5)	Cd(1)-O(11)	2.629(6)
Cd(2)-N(8) ^{#3}	2.235(9)	Cd(2)-N(5)	2.253(10)
Cd(2)-O(6)	2.274(7)	Cd(2)-O(7)	2.300(10)
Cd(2)-O(8)	2.397(8)	Cd(2)-O(5)	2.471(8)
N(1)-Cd(1)-N(4) ^{#1}	107.8(3)	N(1)-Cd(1)-O(12)	128.0(3)
N(4) ^{#1} -Cd(1)-O(12)	105.6(3)	N(1)-Cd(1)-O(2) ^{#2}	134.1(2)
N(4) ^{#1} -Cd(1)-O(2) ^{#2}	87.2(3)	O(12)-Cd(1)-O(2) ^{#2}	85.7(2)
N(1)-Cd(1)-O(1) ^{#2}	90.9(2)	$N(4)^{\#1}$ -Cd(1)-O(1) $^{\#2}$	138.3(3)

O(12)-Cd(1)-O(1) ^{#2}	89.7(2)	$O(2)^{#2}-Cd(1)-O(1)^{#2}$	54.9(3)
N(1)-Cd(1)-O(11)	88.8(2)	N(4) ^{#1} -Cd(1)-O(11)	90.9(2)
O(12)-Cd(1)-O(11)	51.9(2)	O(2) ^{#2} -Cd(1)-O(11)	135.2(2)
O(1) ^{#2} -Cd(1)-O(11)	127.2(3)	N(8) ^{#3} -Cd(2)-N(5)	101.9(4)
N(8) ^{#3} -Cd(2)-O(6)	134.5(4)	N(5)-Cd(2)-O(6)	99.5(4)
N(8) ^{#3} -Cd(2)-O(7)	106.9(4)	N(5)-Cd(2)-O(7)	85.6(4)
O(6)-Cd(2)-O(7)	114.4(4)	N(8) ^{#3} -Cd(2)-O(8)	99.7(4)
N(5)-Cd(2)-O(8)	136.0(4)	O(6)-Cd(2)-O(8)	91.8(3)
O(7)-Cd(2)-O(8)	51.3(4)	N(8) ^{#3} -Cd(2)-O(5)	84.5(3)
N(5)-Cd(2)-O(5)	99.9(3)	O(6)-Cd(2)-O(5)	52.4(3)
O(7)-Cd(2)-O(5)	166.2(4)	O(8)-Cd(2)-O(5)	120.1(4)

Table S6b Hydrogen bonds for 6 (Å and °).

D-H···A	d(D-H)	$d(H \cdots A)$	$d(D \cdots A)$	<(DHA)
$C(38)-H(38B)\cdots O(1)^{\#7}$	0.97	2.59	3.388(17)	139.5
$C(46)-H(46)\cdots O(5)^{\#8}$	0.93	2.30	3.209(18)	166.5
$C(48)-H(48B)\cdots O(6)^{\#9}$	0.97	2.38	3.14(3)	134.4
$C(51)-H(51A)\cdots O(8)^{\#8}$	0.97	2.55	3.23(2)	126.9

^{#1} -x, y+1/2, -z; ^{#2} x-3, y, z-1; ^{#3} -x+3, y+1/2, -z+1; ^{#7} x-2, y, z-1; ^{#8} -x+2, y-1/2, -z+1; ^{#9} x+1, y, z.

Table S7a Selected bond distances (Å) and angles (°) for 7.				
$Zn(1)-O(2)^{\#1}$	1.938(9)	Zn(1)-O(12)	2.011(9)	
Zn(1)-N(1)	2.016(11)	$Zn(1)-N(4)^{\#2}$	2.021(11)	
Zn(2)-O(5)	1.975(9)	Zn(2)-N(5)	1.992(10)	
Zn(2)-O(7)	1.996(11)	$Zn(2)-N(8)^{\#3}$	2.064(10)	
O(2) ^{#1} -Zn(1)-O(12)	105.1(4)	$O(2)^{#1}$ -Zn(1)-N(1)	120.4(4)	
O(12)-Zn(1)-N(1)	118.3(4)	$O(2)^{\#1}$ -Zn(1)-N(4) ^{#2}	97.5(4)	

O(12)-Zn(1)-N(4) ^{#2}	106.7(4)	N(1)-Zn(1)-N(4) ^{#2}	106.1(4)
O(5)-Zn(2)-N(5)	119.1(4)	O(5)-Zn(2)-O(7)	98.4(4)
N(5)-Zn(2)-O(7)	126.5(5)	$O(5)-Zn(2)-N(8)^{\#3}$	104.9(4)
$N(5)-Zn(2)-N(8)^{\#3}$	110.7(4)	O(7)-Zn(2)-N(8) ^{#3}	92.7(5)

Table S7b Hydrogen bonds for **7** (Å and °).

D-H···A	d(D-H)	$d(H \cdots A)$	$d(D \cdots A)$	<(DHA)
$C(27)-H(27)\cdots O(10)^{\#7}$	0.93	2.49	3.392(14)	164.6
$C(30)-H(30)\cdots O(9)^{\#8}$	0.93	2.50	3.421(14)	171.7
$C(38)-H(38B)\cdots O(1)^{\#9}$	0.97	2.46	3.115(17)	125.0
C(41)-H(41A) ···O(12) ^{#10}	0.97	2.57	3.326(16)	134.9
$C(42)-H(42)\cdots O(11)^{\#7}$	0.93	2.40	3.299(16)	163.5

^{#1} x+3, y, z+1; ^{#2} -x, y-1/2, -z+1; ^{#3} -x-3, y+1/2, -z; ^{#7} x-1, y, z; ^{#8} x+1, y, z; ^{#9} x+2, y, z+1; ^{#10} -x+1, y+1/2, -z+1.

Table S8a	Selected bond	distances (Å) and angles	(°) for 8 .
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$Cd(1)-N(4)^{\#1}$	2.237(4)	$Cd(1)-O(5)^{#2}$	2.265(3)	
Cd(1)-N(1)	2.281(4)	Cd(1)-O(2)	2.297(3)	
Cd(1)-O(1)	2.456(3)	$Cd(1)-O(6)^{#2}$	2.530(3)	
$N(4)^{\#1}$ -Cd(1)-O(5) $^{\#2}$	123.76(13)	N(4) ^{#1} -Cd(1)-N(1)	106.66(15)	
O(5) ^{#2} -Cd(1)-N(1)	111.21(13)	N(4) ^{#1} -Cd(1)-O(2)	134.03(13)	
O(5) ^{#2} -Cd(1)-O(2)	91.12(13)	N(1)-Cd(1)-O(2)	82.95(12)	
N(4) ^{#1} -Cd(1)-O(1)	87.26(13)	O(5) ^{#2} -Cd(1)-O(1)	102.45(12)	
N(1)-Cd(1)-O(1)	125.16(12)	O(2)-Cd(1)-O(1)	53.76(11)	
$N(4)^{\#1}$ -Cd(1)-O(6) $^{\#2}$	87.53(12)	O(5) ^{#2} -Cd(1)-O(6) ^{#2}	54.17(11)	
N(1)-Cd(1)-O(6) ^{#2}	88.85(12)	O(2)-Cd(1)-O(6) ^{#2}	138.26(11)	
O(1)-Cd(1)-O(6) ^{#2}	145.58(11)			

Symmetry transformations used to generate equivalent atoms:

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2.242(6)	$Cd(1)-O(5)^{\#1}$	2.263(5)
2.284(5)	Cd(1)-O(2)	2.293(5)
2.456(5)	$Cd(1)-O(6)^{\#1}$	2.535(5)
123.7(2)	N(1)-Cd(1)-N(5) ^{#2}	106.5(2)
111.29(19)	N(1)-Cd(1)-O(2)	134.22(19)
91.40(19)	N(5) ^{#2} -Cd(1)-O(2)	82.49(18)
87.5(2)	O(5) ^{#1} -Cd(1)-O(1)	102.45(18)
125.08(17)	O(2)-Cd(1)-O(1)	54.02(16)
87.16(19)	$O(5)^{\#1}$ -Cd(1)-O(6)^{\#1}	54.16(17)
89.17(17)	O(2)-Cd(1)-O(6) ^{#1}	138.48(17)
145.36(16)		
	2.242(6) 2.284(5) 2.456(5) 123.7(2) 111.29(19) 91.40(19) 87.5(2) 125.08(17) 87.16(19) 89.17(17) 145.36(16)	$2.242(6)$ $Cd(1)-O(5)^{\#1}$ $2.284(5)$ $Cd(1)-O(2)$ $2.456(5)$ $Cd(1)-O(6)^{\#1}$ $123.7(2)$ $N(1)-Cd(1)-N(5)^{\#2}$ $111.29(19)$ $N(1)-Cd(1)-O(2)$ $91.40(19)$ $N(5)^{\#2}-Cd(1)-O(2)$ $87.5(2)$ $O(5)^{\#1}-Cd(1)-O(1)$ $125.08(17)$ $O(2)-Cd(1)-O(1)$ $87.16(19)$ $O(5)^{\#1}-Cd(1)-O(6)^{\#1}$ $89.17(17)$ $O(2)-Cd(1)-O(6)^{\#1}$ $145.36(16)$ $O(5)^{\#1}-Cd(1)-O(6)^{\#1}$

Table S9a Selected bond distances (Å) and angles (°) for 9.

Symmetry transformations used to generate equivalent atoms:

^{#1} -x+3/2, -y+2, z+1/2; ^{#2} x+3/2, -y+3/2, -z+1.

Table S10a Selected bond distances (Å) and angles (°) for 10.				
Cd(1)-O(5)	2.205(3)	Cd(1)-N(1)	2.235(4)	
$Cd(1)-N(4)^{\#1}$	2.254(3)	Cd(1)-O(1) ^{#2}	2.306(3)	
$Cd(1)-O(2)^{\#2}$	2.456(4)			
O(5)-Cd(1)-N(1)	120.69(13)	O(5)-Cd(1)-N(4) ^{#1}	101.15(12)	
N(1)-Cd(1)-N(4) ^{#1}	102.78(13)	O(5)-Cd(1)-O(1) ^{#2}	135.17(12)	
N(1)-Cd(1)-O(1) ^{#2}	87.17(13)	$N(4)^{\#1}$ -Cd(1)-O(1) $^{\#2}$	106.02(15)	
O(5)-Cd(1)-O(2) ^{#2}	88.49(13)	N(1)-Cd(1)-O(2) ^{#2}	139.90(12)	
$N(4)^{\#1}-Cd(1)-O(2)^{\#2}$	96.94(14)	$O(1)^{#2}-Cd(1)-O(2)^{#2}$	53.69(12)	

Symmetry transformations used to generate equivalent atoms:

^{#1} x+3/2, -y+3/2, -z+1; ^{#2} -x+3/2, -y+2, z-1/2.

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Fig. S1 Coordination environment of the Co(II) ions in 2 with the hydrogen atoms omitted for clarity (30% probability displacement ellipsoids). Symmetry code: $^{#1}$ -x, y-1/2, -z.



Fig. S2 View of the 3D supramolecular structure connected by hydrogen bonds of compound 5.



Fig. S3 ORTEP view of **7** showing the local coordination environment of Zn(II) atom with hydrogen atoms omitted for clarity (30% probability displacement ellipsoids). Symmetry codes: ^{#1} x+3, y, z+1; ^{#2} -x, y-1/2, -z+1; ^{#3} -x-3, y+1/2, -z.



Fig. S4 View of the 3D frameworks of compound 8.



Fig. S5 ORTEP view of **9** showing the local coordination environment of Cd(II) atom with hydrogen atoms omitted for clarity (30% probability displacement ellipsoids). Symmetry codes: $^{\#1}$ -x+3/2, -y+2, z+1/2; $^{\#2}$ x+3/2, -y+3/2, -z+1.



Fig. S6 ORTEP view of **10** showing the local coordination environment of Cd(II) atom with hydrogen atoms omitted for clarity (30% probability displacement ellipsoids). Symmetry codes: $^{#1}$ x+3/2, -y+3/2, -z+1; $^{#2}$ -x+3/2, -y+2, z-1/2.



Fig. S7 The simulated (blue) and experimental (black) XRD patterns for 1-10.



Fig. S8 The TGA curves of compounds 1–10.