Electronic Supplementary Information (ESI) for

Novel noncentrosymmetric polar coordination compounds derived from chiral histidine ligands, (L– and D–Histidine)$ZnBr_3$ and (L– and D–Histidine)$_2Cd_2Cl_5$

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Table of contents

Figure S1. Experimental and calculated powder X-ray diffraction patterns of **L–ZnBr** and **D–ZnBr**.

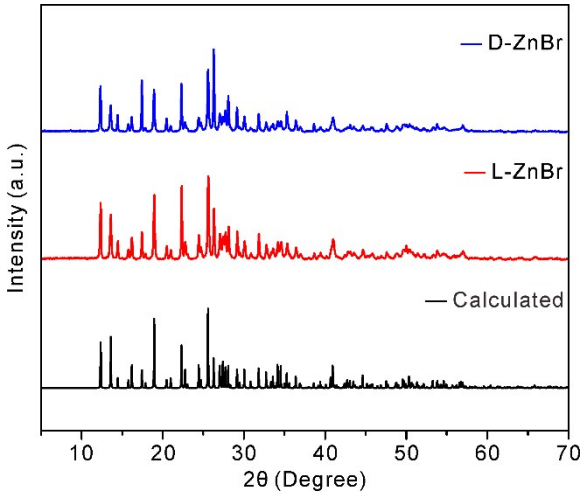


Figure S2. Experimental and calculated powder X-ray diffraction patterns of **L–CdCl** and **D–CdCl**.

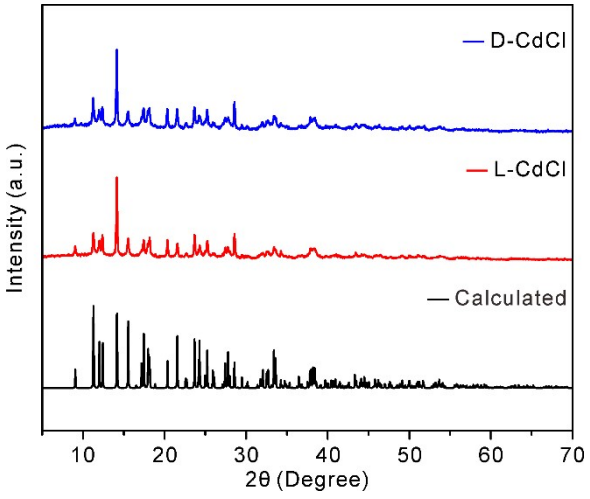
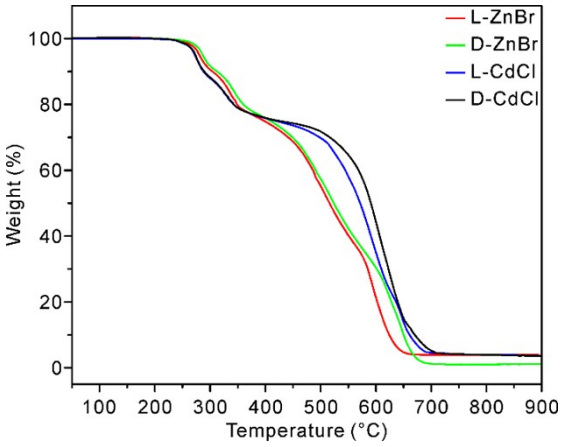


Figure S3. TGA diagrams for **L–ZnBr**, **D–ZnBr**, **L–CdCl**, and **D–CdCl**.



Upon further heating, weight losses attributed to the decomposition of coordinated histidine in the title compounds are observed. Compounds **L–ZnBr** and **D–ZnBr** further decompose to ZnO. The thermal decomposition can be represented by the following reaction:

$8(C_6H_{10}N_3O_2ZnBr_3) + 45O_2 \rightarrow 48CO_2 + 8H_2O + 24NH_3 + 6ZnBr_2 + 2ZnO + 6Br_2$

The experimental values of 3.9% and 2.5% for the decomposed residues of compounds **L–ZnBr** and **D–ZnBr**, respectively, match well with the theoretical value, 4.4%.

Similarly, Compounds **L–CdCl** and **D–CdCl** decompose to CdO, in which the thermal decomposition can be written as the following reaction:

$8(C_{12}H_{20}N_6O_4Cd_2Cl_6) + 85O_2 \rightarrow 96CO_2 + 8H_2O + 48NH_3 + 14CdCl_2 + 2CdO + 10Cl_2$

The experimental values of 4.5% and 4.3% for the decomposed residues of compounds **L–CdCl** and **D–CdCl**, respectively, match well with the theoretical value, 4.3%.

Figure S4. Powder X-ray diffraction patterns for calcined products of **ZnBr** and **CdCl**.

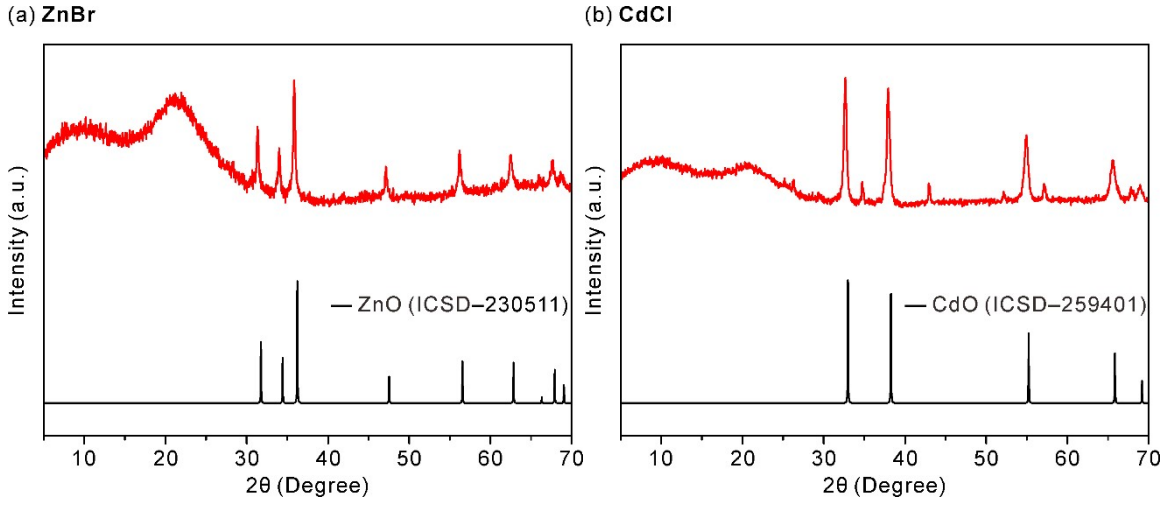


Figure S5. IR spectra for **L–ZnBr**, **D–ZnBr**, **L–CdCl**, and **D–CdCl**.

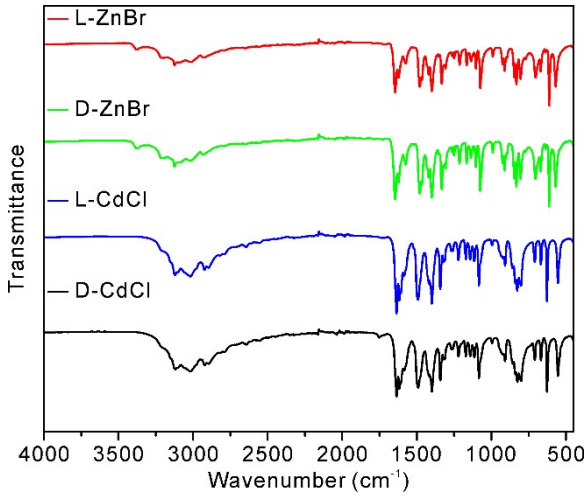


Figure S6. UV-vis spectra for L–histidine, D–histidine, **L–ZnBr**, **D–ZnBr**, **L–CdCl**, and **D–CdCl**.

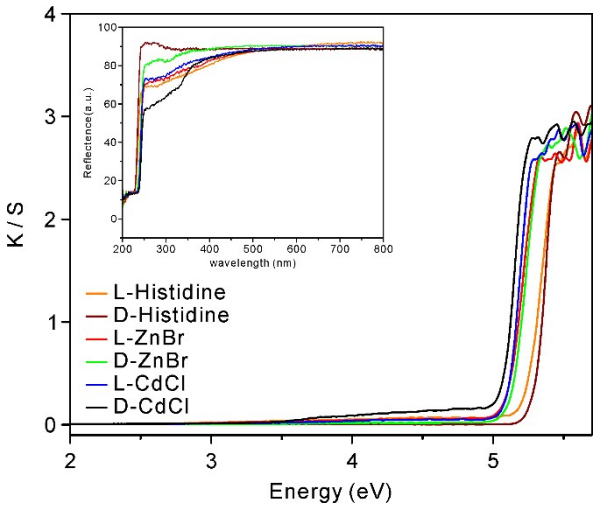


Figure S7. Total and partial density of state for (a) **D–ZnBr** and (b) **D–CdCl**.

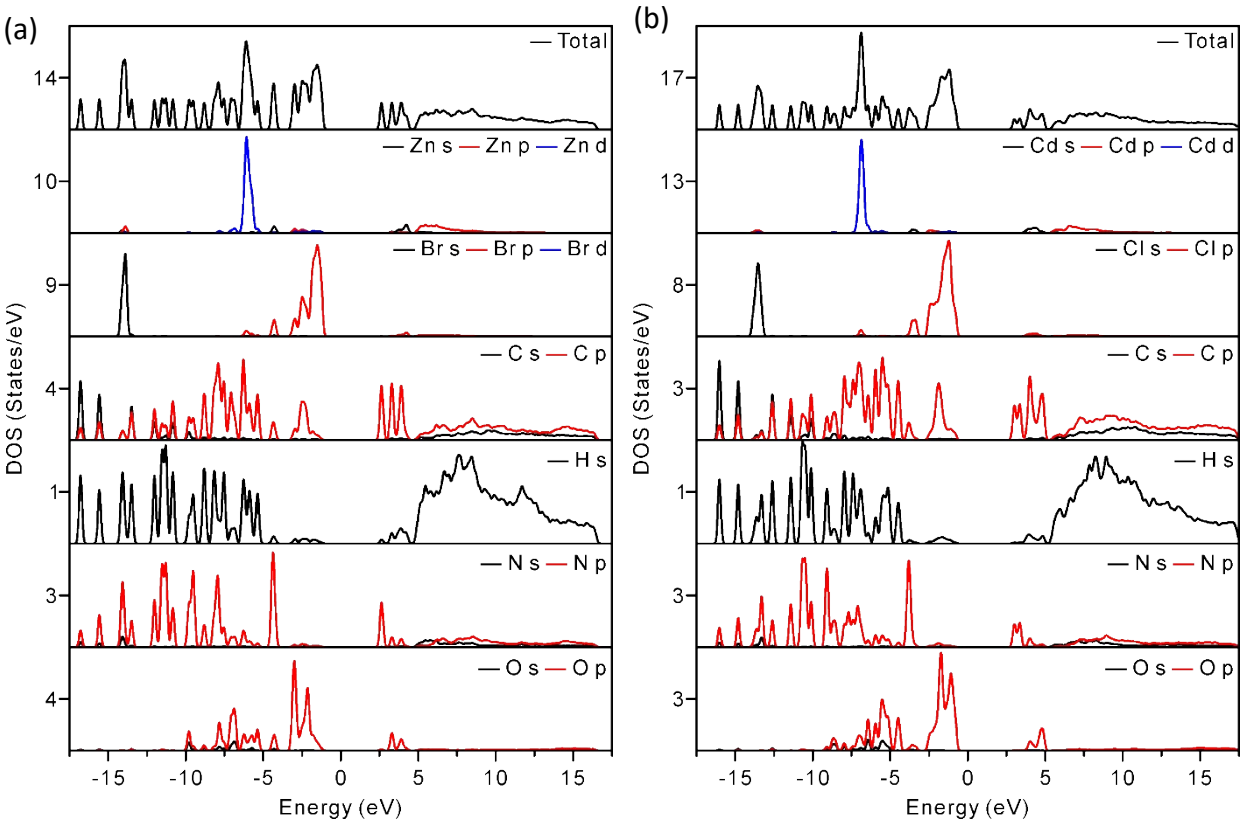


Figure S8. Band structures for **L–ZnBr**, **D–ZnBr**, **L–CdCl**, and **D–CdCl**.

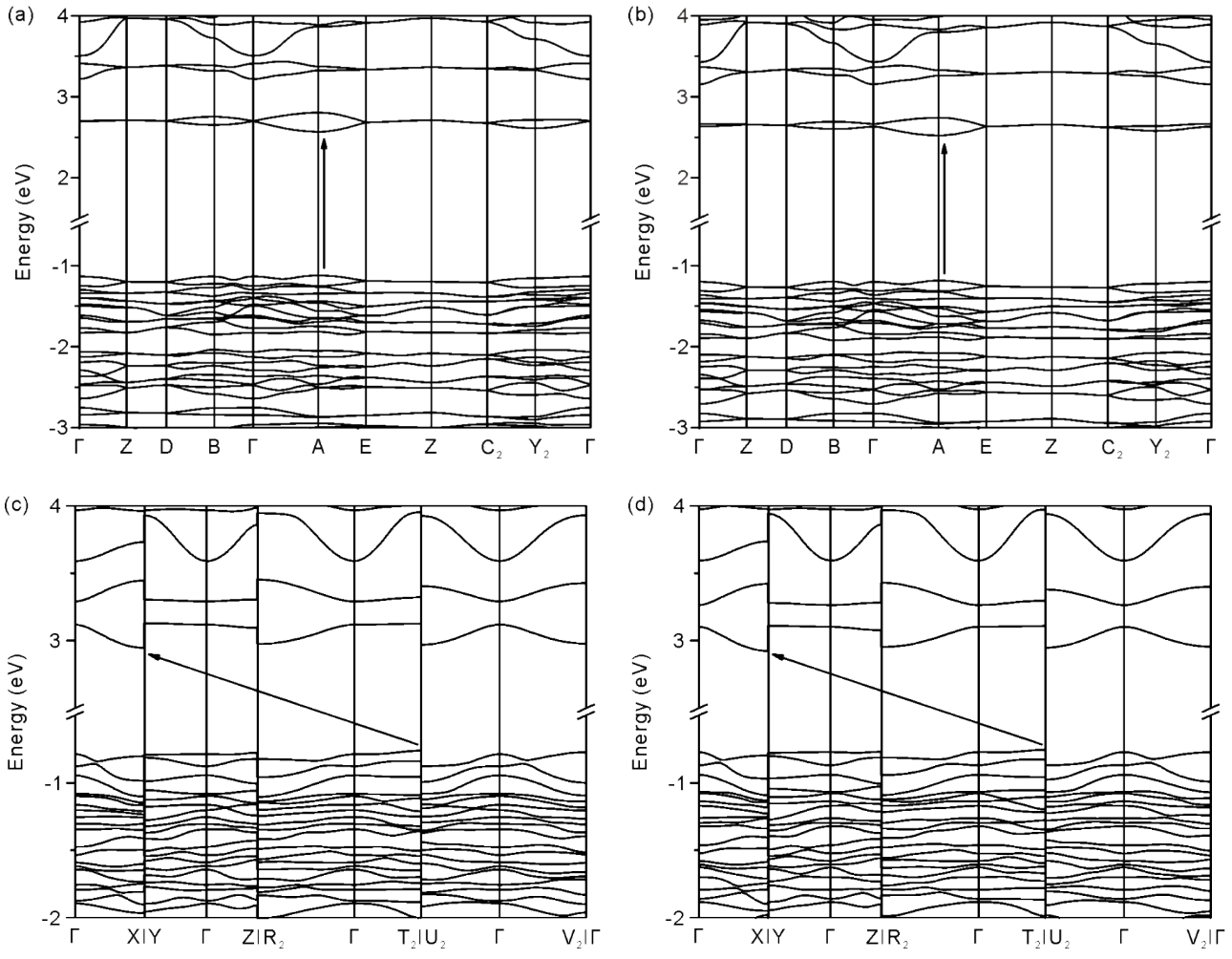


Figure S9. Net moments and dipole moments of [$ZnOBr_3$] and [$CdOCl_4$] polyhedra in a unit cell for (a) **L–ZnBr** and (b) **L–CdCl**, respectively.

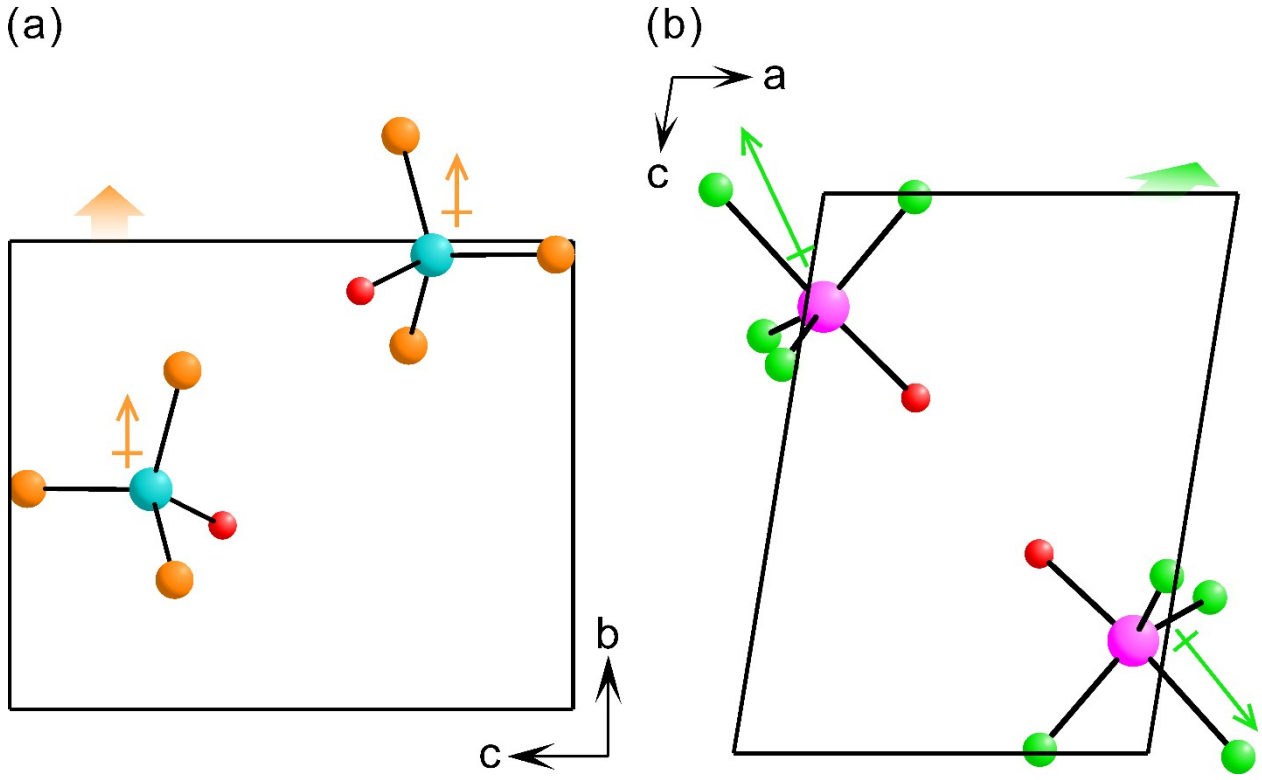
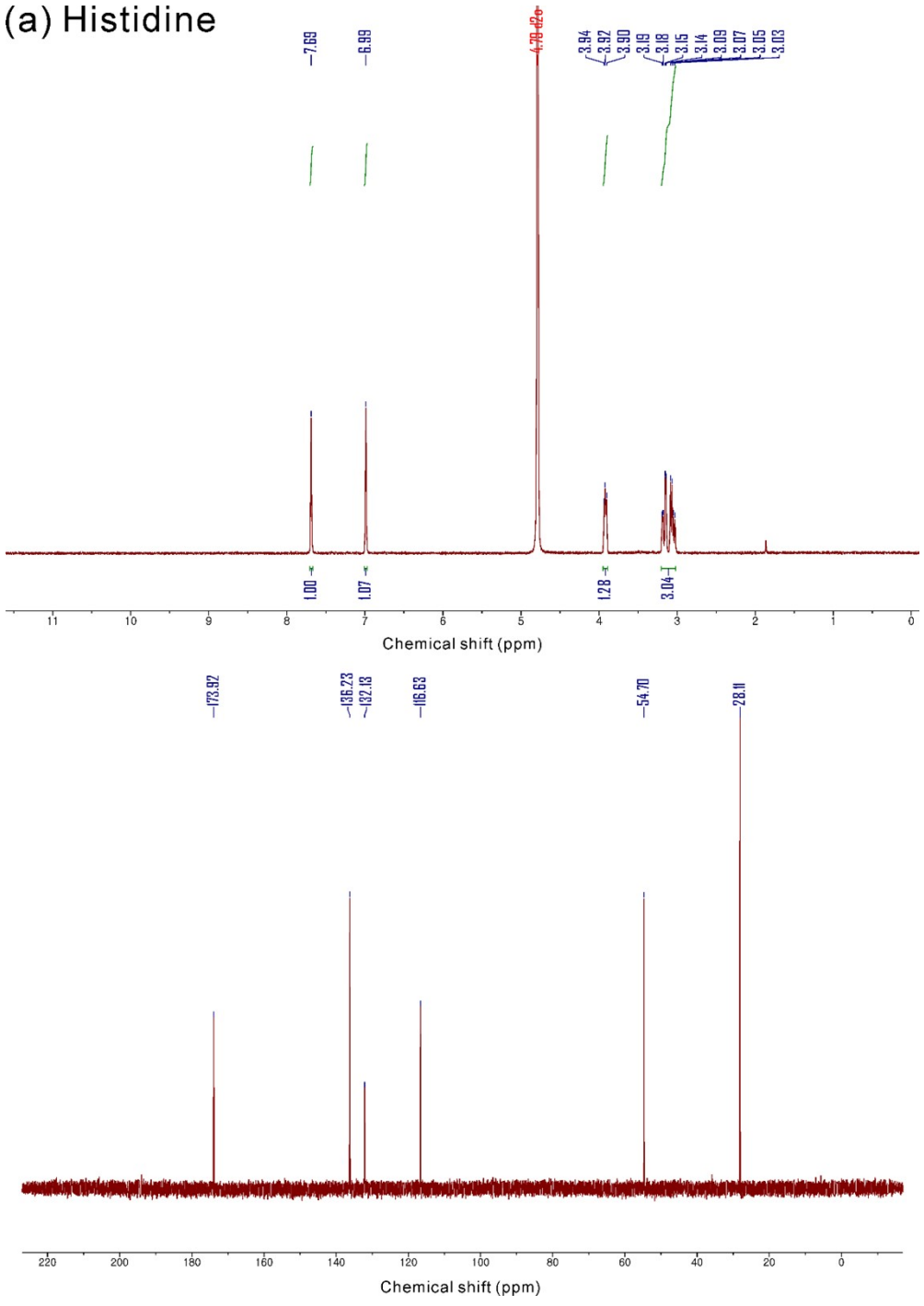
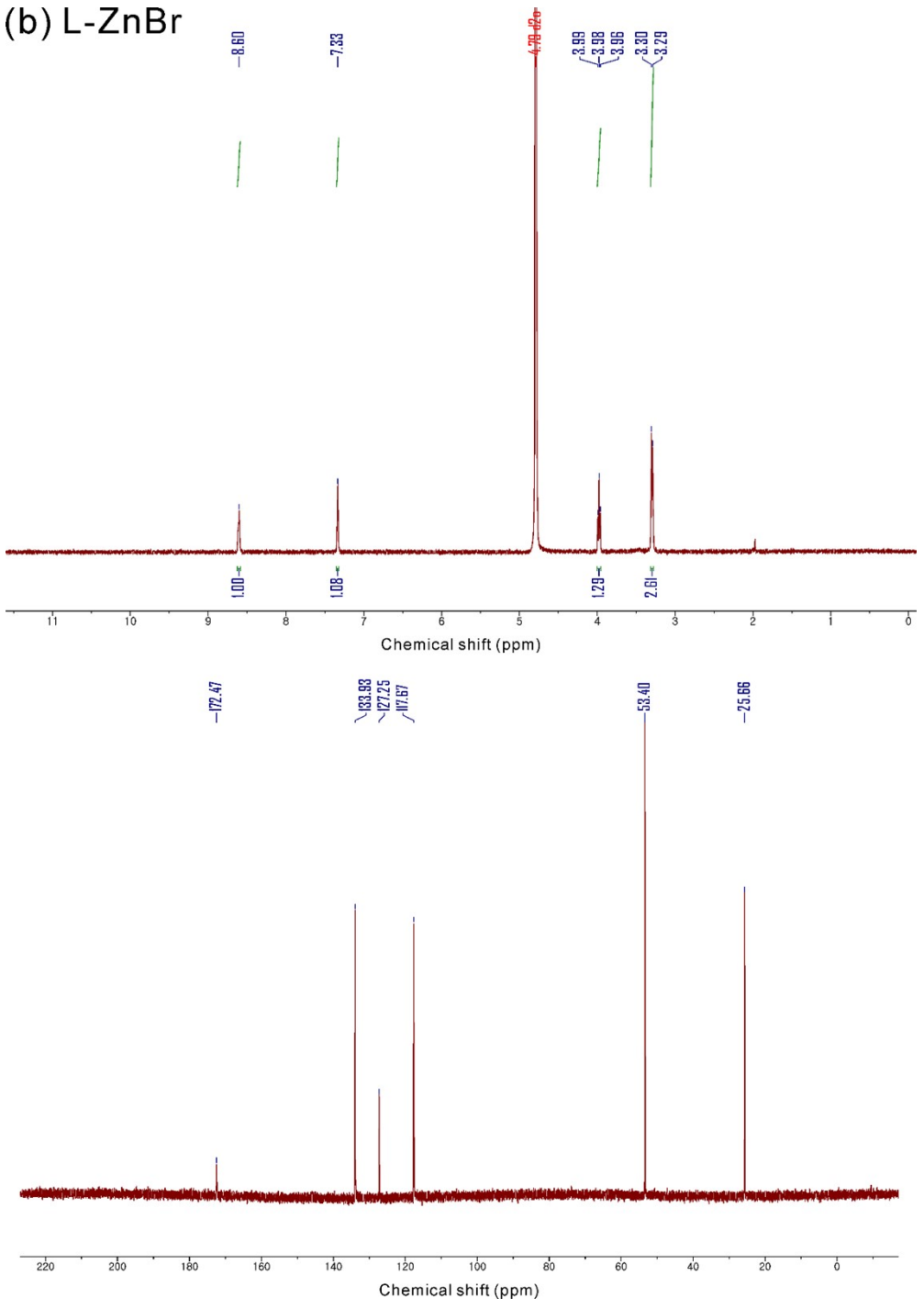


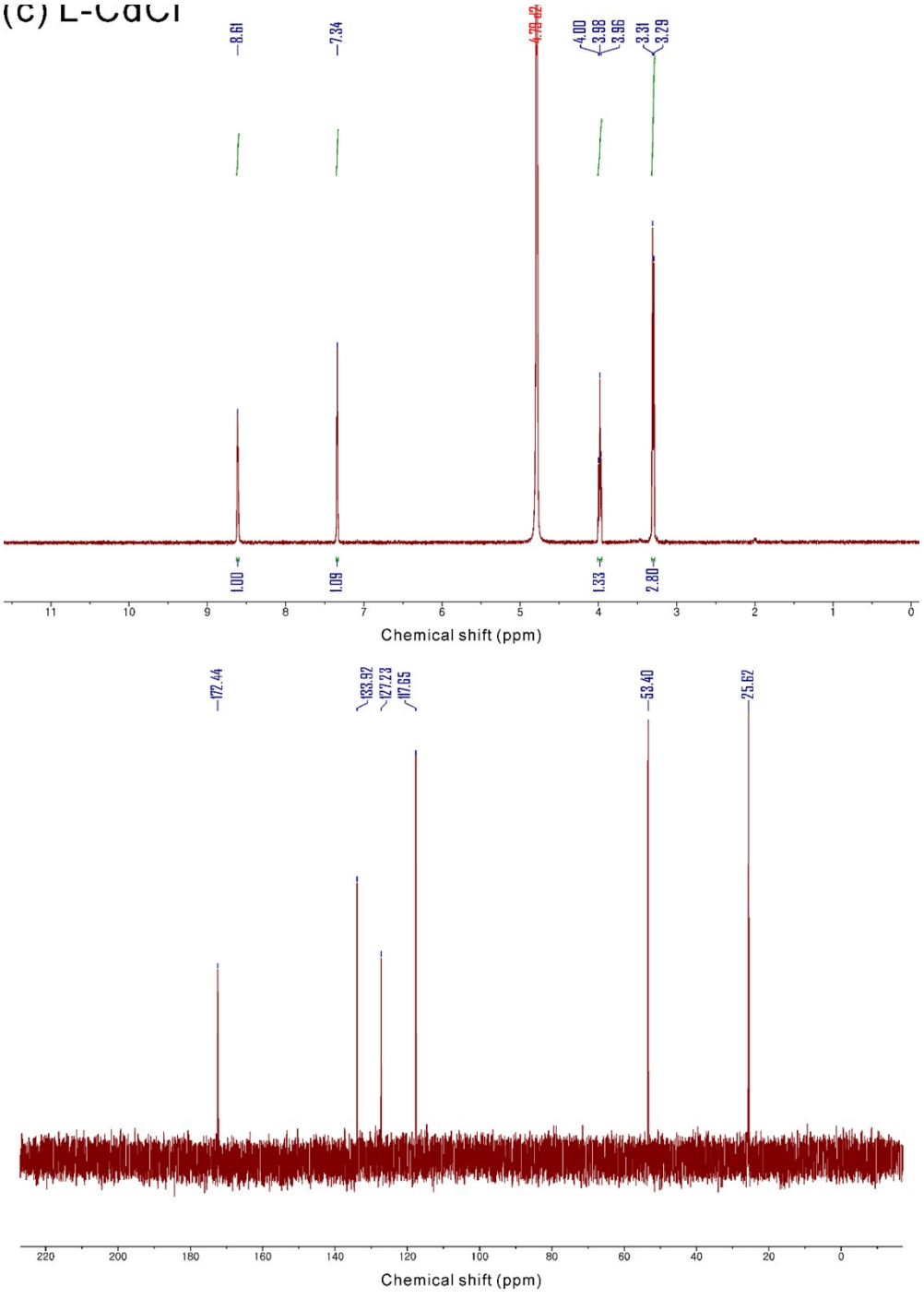
Figure S10. ^{1}H NMR (400 MHz, D_2O, room temperature) and ^{13}C NMR (100 MHz, D_2O, room temperature) spectra for (a) histidine, (b) **L-ZnBr**, and (c) **L-CdCl**.



^{1}H NMR (400 MHz, D_2O): δ 7.69 (s, 1 H), δ 6.99 (s, 1 H), δ 3.94–3.90 (t, 1 H), δ 3.19–3.03 (m, 3 H)
^{13}C NMR (100 MHz, D_2O): δ173.92, 136.23, 132.13, 116.63, 54.70, 28.11 ppm



^{1}H NMR (400 MHz, D_2O): δ 8.60 (s, 1 H), δ 7.33 (s, 1 H), δ 3.99–3.96 (t, 1 H), δ 3.30–3.29 (d, 3 H)
^{13}C NMR (100 MHz, D_2O): δ172.47, 133.93, 127.25, 117.67, 53.40, 25.66 ppm



^{1}H NMR (400 MHz, D_2O): δ 8.61 (s, 1 H), δ 7.34 (s, 1 H), δ 4.00–3.96 (t, 1 H), δ 3.31–3.29 (d, 3 H)
^{13}C NMR (100 MHz, D_2O): δ 172.44, 133.92, 127.23, 117.65, 53.40, 25.62 ppm

Table S1. Crystallographic Data for **L-ZnBr**, **D-ZnBr**, **L-CdCl**, and **D-CdCl**.

compound	**L-ZnBr**	**D-ZnBr**	**L-CdCl**	**D-CdCl**
formula	$C_6H_{10}N_3O_2ZnBr_3$		$C_{12}H_{20}N_6O_4Cd_2Cl_6$	
Fw	461.27	461.27	749.84	749.84
space group	$P2_1$	$P2_1$	$P1$	$P1$
a (Å)	7.1916(3)	7.1874(6)	7.2513(4)	7.2590(5)
b (Å)	8.4614(4)	8.4578(8)	8.3073(5)	8.3140(5)
c (Å)	10.2086(5)	10.1952(9)	10.3629(6)	10.3712(6)
α (°)	90	90	107.6430(10)	107.6460(10)
β (°)	95.1770(10)	95.224(3)	96.907(2)	96.894(2)
γ (°)	90	90	95.774(2)	95.746(2)
V (Å^3)	618.67(5)	617.19(10)	584.34(6)	585.96(6)
Z	2	2	1	1
T (K)	296(2)	296(2)	296(2)	296(2)
λ (Å)	0.71073	0.71073	0.71073	0.71073
ρ_{calcd} (g/ cm^{-3})	2.476	2.482	2.131	2.125
$R(F_o)^a$	0.0230	0.0369	0.0153	0.0187
$R_w(F_o^2)^b$	0.0544	0.0820	0.0393	0.0460
Flack x	0.046(4)	0.028(7)	0.009(7)	-0.009(10)

$^a R(F) = \sum||F_o| - |F_c||/\sum|F_o|$,

$^b R_w(F_o^2) = \{\sum w[(F_o)^2 - (F_c)^2]^2/\sum w[(F_o)^2]^2\}^{1/2}$.

Table S2. Selected distances (Å) for **L–ZnBr**.

Zn(1)–O(1)	2.013(3)	C(2)–N(1)	1.490(6)
Zn(1)–Br(2)	2.3718(7)	C(2)–C(3)	1.536(6)
Zn(1)–Br(3)	2.3942(7)	C(3)–C(4)	1.490(6)
Zn(1)–Br(1)	2.4135(8)	C(4)–C(5)	1.351(7)
C(1)–O(2)	1.231(6)	C(4)–N(2)	1.380(6)
C(1)–O(1)	1.270(6)	C(5)–N(3)	1.358(8)
C(1)–C(2)	1.530(5)	C(6)–N(2)	1.330(7)
		C(6)–N(3)	1.331(8)

Table S3. Selected distances (Å) for **D–ZnBr**.

Zn(1)–O(1)	2.009(5)	C(2)–N(1)	1.497(9)
Zn(1)–Br(2)	2.3709(12)	C(2)–C(3)	1.523(10)
Zn(1)–Br(3)	2.3949(12)	C(3)–C(4)	1.484(10)
Zn(1)–Br(1)	2.4116(14)	C(4)–C(5)	1.354(11)
C(1)–O(2)	1.238(9)	C(4)–N(2)	1.377(10)
C(1)–O(1)	1.259(9)	C(5)–N(3)	1.336(13)
C(1)–C(2)	1.511(9)	C(6)–N(3)	1.314(13)
		C(6)–N(2)	1.343(12)

Table S4. Selected distances (Å) for **L–CdCl**.

Cd(1)–O(1)	2.324(3)	C(1)-O(2)	1.240(6)	C(7)–O(4)	1.226(6)
Cd(1)–Cl(2)	2.4731(11)	C(1)-O(1)	1.267(6)	C(7)–O(3)	1.266(6)
Cd(1)–Cl(1)	2.4851(11)	C(1)-C(2)	1.532(7)	C(7)–C(8)	1.545(6)
Cd(1)–Cl(3)	2.5092(12)	C(2)-N(1)	1.491(5)	C(8)–N(4)	1.478(6)
Cd(1)–Cl(5)	2.7660(12)	C(2)-C(3)	1.523(6)	C(8)–C(9)	1.534(6)
Cd(2)–O(3)	2.371(3)	C(3)–C(4)	1.492(6)	C(9)–C(10)	1.492(7)
Cd(2)–Cl(6)	2.4525(12)	C(4)-C(5)	1.356(6)	C(10)–C(11)	1.346(7)
Cd(2)–Cl(5)	2.4985(12)	C(4)-N(2)	1.375(6)	C(10)–N(5)	1.379(6)
Cd(2)–Cl(4)	2.5170(11)	C(5)-N(3)	1.364(7)	C(11)–N(6)	1.392(7)
Cd(2)–Cl(3)	2.7510(12)	C(6)-N(2)	1.309(7)	C(12)–N(6)	1.312(8)
		C(6)-N(3)	1.320(8)	C(12)–N(5)	1.338(6)

Table S5. Selected distances (Å) for **D–CdCl**.

Cd(1)-O(1)	2.329(3)	C(1)-O(2)	1.239(6)	C(7)-O(4)	1.231(6)
Cd(1)-Cl(2)	2.4735(12)	C(1)-O(1)	1.264(6)	C(7)-O(3)	1.277(6)
Cd(1)-Cl(1)	2.4891(11)	C(1)-C(2)	1.544(6)	C(7)-C(8)	1.536(7)
Cd(1)-Cl(3)	2.5093(13)	C(2)-N(1)	1.488(6)	C(8)-N(4)	1.484(6)
Cd(1)-Cl(5)	2.7718(12)	C(2)-C(3)	1.529(7)	C(8)-C(9)	1.532(7)
Cd(2)-O(3)	2.370(3)	C(3)-C(4)	1.497(7)	C(9)-C(10)	1.495(7)
Cd(2)-Cl(6)	2.4559(12)	C(4)-C(5)	1.357(7)	C(10)-C(11)	1.352(7)
Cd(2)-Cl(5)	2.5003(13)	C(4)-N(2)	1.370(7)	C(10)-N(5)	1.361(7)
Cd(2)-Cl(4)	2.5180(11)	C(5)-N(3)	1.366(7)	C(11)-N(6)	1.369(7)
Cd(2)-Cl(3)	2.7534(12)	C(6)-N(3)	1.304(8)	C(12)-N(6)	1.324(8)
		C(6)-N(2)	1.329(7)	C(12)-N(5)	1.335(7)

Table S6. Hydrogen bond distances (Å) for **L–ZnBr**, **D–ZnBr**, **L–CdCl**, and **D–CdCl**.

Hydrogen bond distances (Å)			
Name	D–H···A	d(H···A)	d(D···A)
L–ZnBr	N(2)–H(2N)···O(2)#1	2.07	2.832(6)
	N(1)–H(1B)···O(1)#2	2.09	2.974(6)
Symmetry operation: #1 -x+1,y-1/2,-z+1 ; #2 -x+1,y+1/2,-z+1			
Hydrogen bond distances (Å)			
D–ZnBr	N(2)–H(2N)···O(2)#1	2.07	2.830(9)
	N(1)–H(1C)···O(1)#2	2.10	2.981(9)
Symmetry operation: #1 -x+1,y+1/2,-z+1 #2 -x+1,y-1/2,-z+1			

Hydrogen bond distances (Å)			
Name	D–H···A	d(H···A)	d(D···A)
L–CdCl	N(2)-H(2N)···O(4)#1	1.96	2.722(5)
	N(1)-H(1B)···O(3)#2	1.99	2.873(5)
	N(5)-H(5N)···O(2)#3	2.00	2.766(5)
	N(4)-H(4B)···O(1)#4	2.06	2.923(5)
Symmetry operation: #1 x+1,y,z+1; #2 x+1,y+1,z+1; #3 x-1,y-1,z-1; #4 x-1,y,z-1			
Hydrogen bond distances (Å)			
Name	D–H···A	d(H···A)	d(D···A)
D–CdCl	N(2)-H(2N)···O(4)#1	1.95	2.714(5)
	N(1)-H(1C)···O(3)#2	1.99	2.871(5)
	N(5)-H(5N)···O(2)#3	2.01	2.771(5)
	N(4)-H(4C)···O(1)#4	2.06	2.927(5)
Symmetry operation: #1 x-1,y,z-1; #2 x-1,y-1,z-1; #3 x+1,y+1,z+1; #4 x+1,y,z+1			