Supporting Information

Acentric and Chiral 4-Connected Metal-Organic Frameworks based on Racemic Chiral Binaphthol-like Ligand of 4-(1-H*(or Methyl)*-imidaozol-1-yl)benzoic acid

Ke-Hui Cui, Shi-Yan Yao, Hai-Qin Li, Yan-Tao Li, Chun-Jie Jiang, Yun-Qi Tian**

* Corresponding author. E-mail: yqtian@lnnu.edu.cn. jiangcj@lnnu.edu.cn. Fax: 86-411-82156989. Tel: 86-411-82159141

Institute of Chemistry for Functionalized Materials, College of Chemistry and Chemical Engineering, Liaoning Normal University, 116029 Dalian, PR CHINA.

Table S1 Crystallographic Data and Structure Refinement Summary for HIBA and HMIBA

	HIBA	HMIBA.
Formula	$C_{10}H_{11}ClN_2O_3$	$C_{11}H_{13}ClN_2O_3$
Fw	242.66	256.68
Crystal systerm	Triclinic	Monoclinic
Space group	*P*-1	$P2_1/c$
a (Å)	7.201(2)	14.465(8)
b (Å)	7.382(2)	7.830(4)
c (Å)	11.328(3)	11.406(6)
α (deg)	77.121(3)	90
β (deg)	77.612(2)	111.139(6)
γ (deg)	75.969(3)	90
V (Å3)	561.2(6)	1205.0(11)
Z	2	4
$D_{calcd.}$	1.424	1.415
Reflections collected / unique	3495/2574	7083/2826
GOF	1.056	1.037
Final *R* indices [*I*>2sigma(*I*)]	R_1=0.0731, wR_2 = 0.2171	R_1 = 0.0522, wR_2 = 0.1393

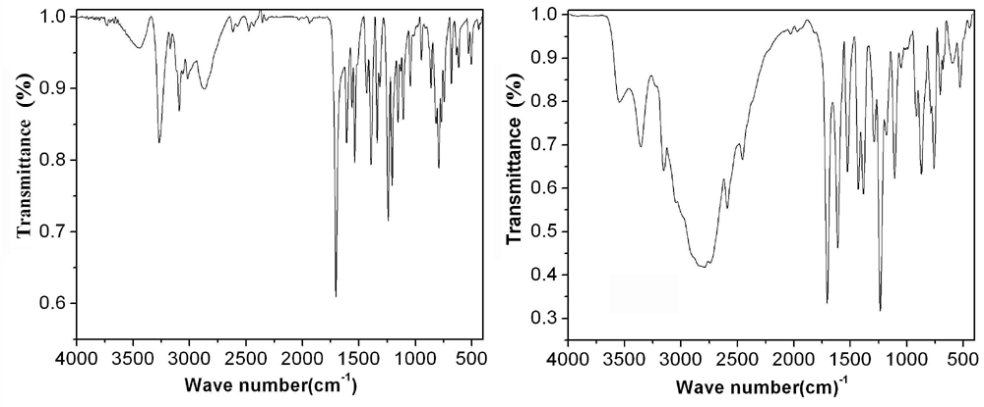

Figure S1 FT-IR of HIBA and HMIBA.

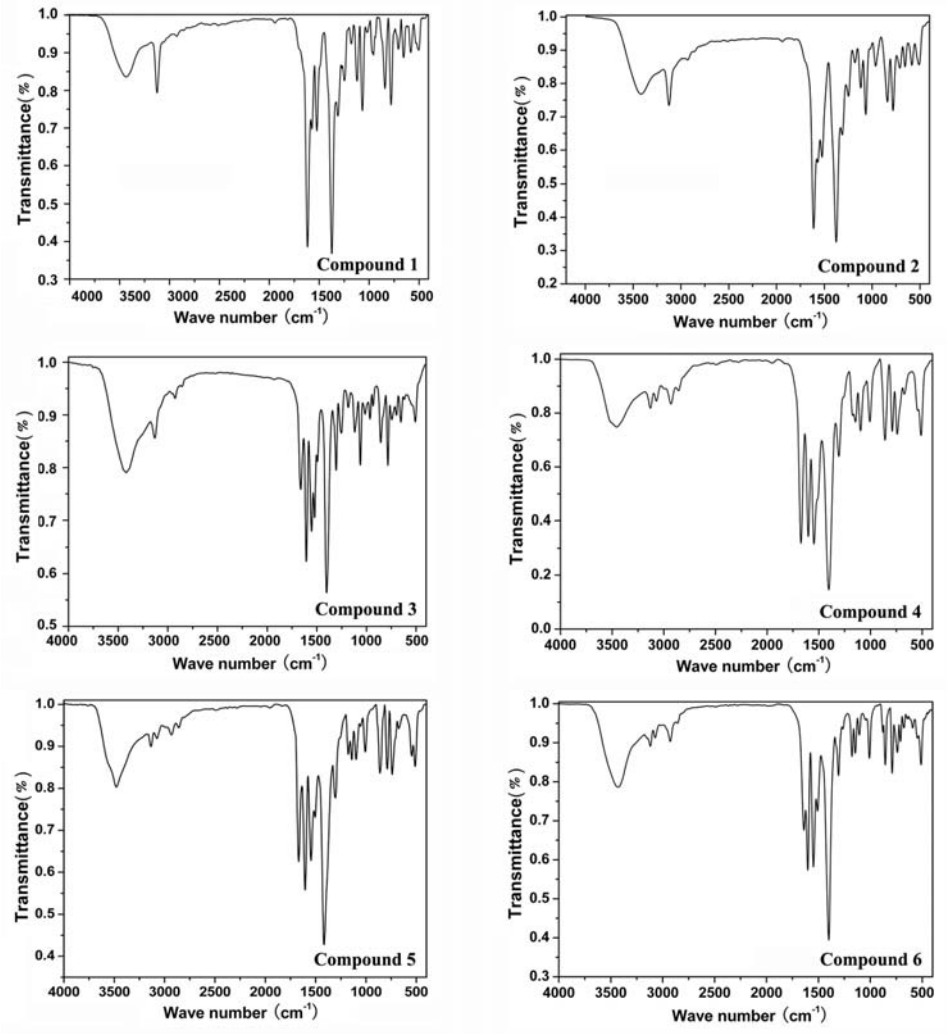

Figure S2 FT-IR of compounds **1**–**6**.

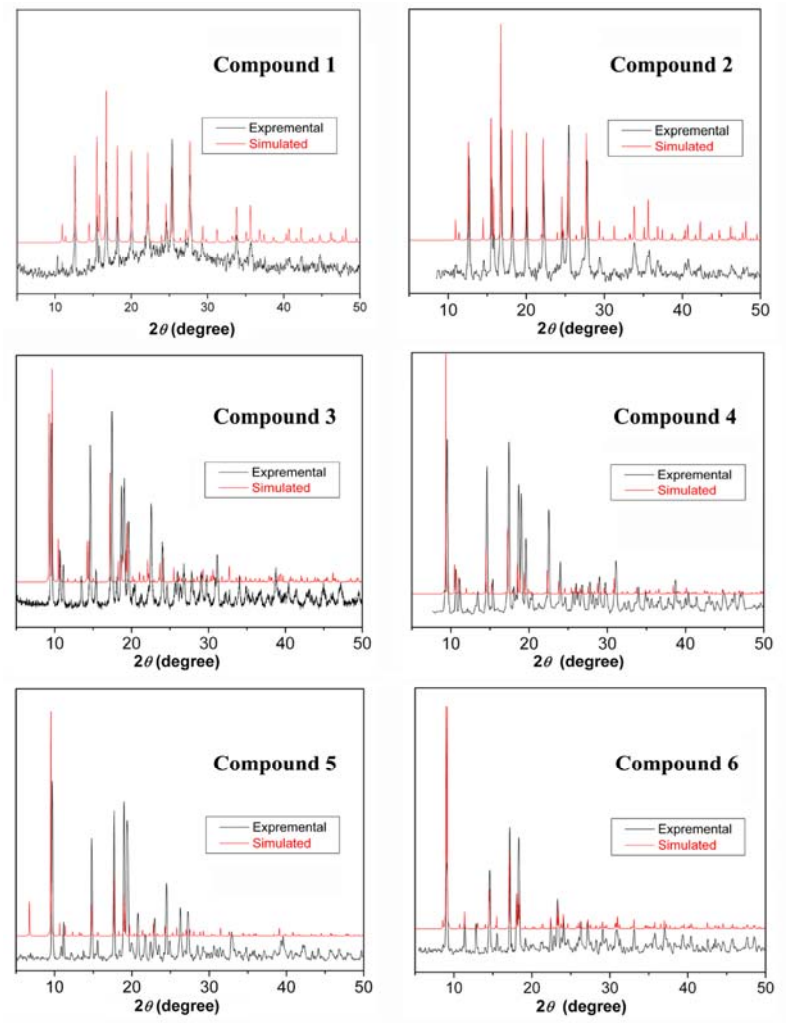

Figure S3 PXRD patterns of compounds **1**–**6**..

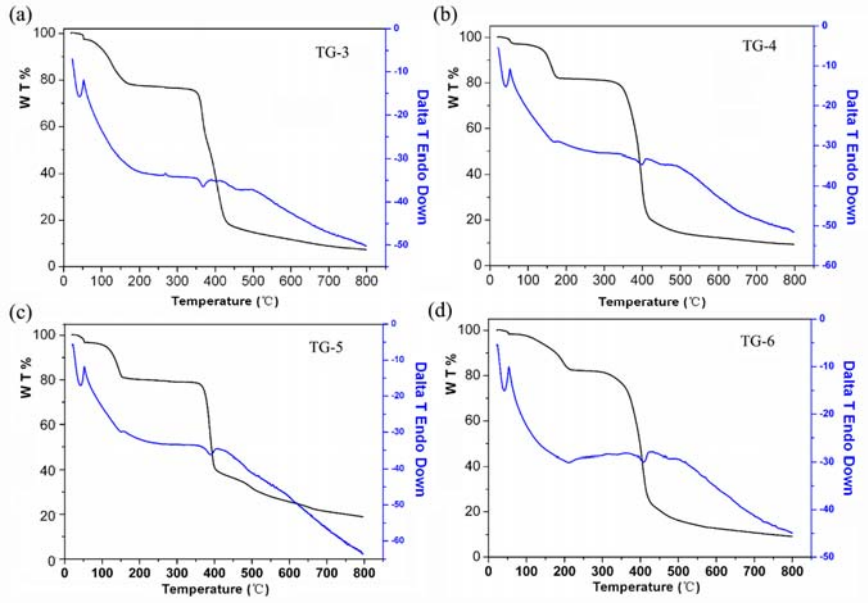

Figure S4. DTA-TGA curves of compounds **3**–**6**

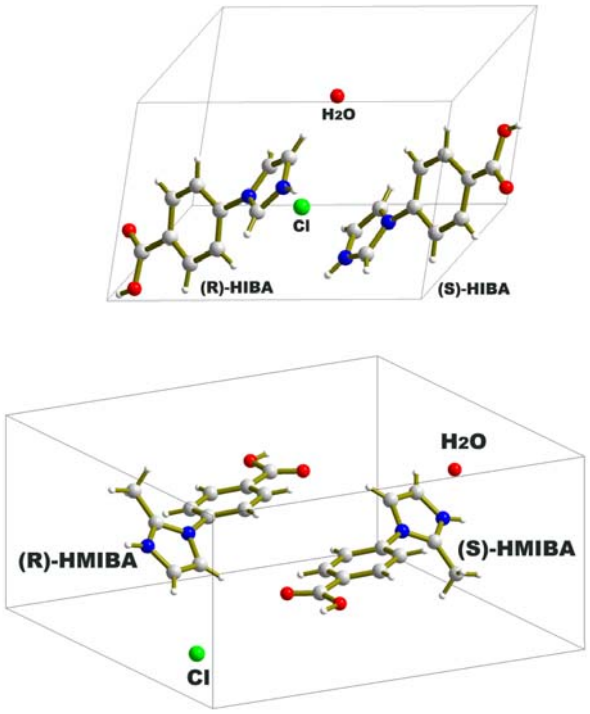

Figure S5 Crystal structures of racemic chiral ligands of HIBA and HMIBA (only a pair of enantiomers are depicted in each of the unit-cell).

Table S2 Selected bond lengths (Å) and angles (°) for 1–6

Compound **1**[a]			
Zn(1)–O(1)#1	1.929(3)	Zn(1)–N(1)#3	2.020(4)
Zn(1)–O(1)#2	1.929(3)	Zn(1)–N(1)	2.020(4)
O(1)#1–Zn(1)–O(1)#2	102.4(2)	O(1)#1–Zn(1)–N(1)#3	110.02(15)
O(1)#1–Zn(1)–N(1)	117.31(14)	O(1)#2–Zn(1)–N(1)#3	117.31(14)
O(1)#2–Zn(1)–N(1)	110.02(15)	N(1)–Zn(1) –N(1)#3	100.5(2)
Compound **2**[b]			
Co(1)–O(1)#1	1.9314(19)	Co(1)–N(1)#3	2.020(2)

Co(1)–O(1)#2	1.9314(19)	Co(1)–N(1)	2.020(2)
O(1)#1–Co(1)–O(1)#2	100.12(15)	O(1)#1–Co(1)–N(1)	118.19(9)
O(1)#1–Co(1)–N(1)#3	110.63(9)	O(1)#2–Co(1)–N(1)	110.63(9)
O(1)#2–Co(1)–N(1)#3	118.19(9)	N(1)#3–Co(1)–N(1)	100.07(13)

Compound **3**[c]

Cd(1)–N(3)	2.242(3)	Cd(1)–O(4)#2	2.334(3)
Cd(1)–N(1)	2.262(3)	Cd(1)–O(2)#1	2.365(3)
Cd(1)–O(1)#1	2.325(2)	Cd(1)–O(3)#2	2.379(3)
N(3)–Cd(1)–N(1)	112.54(14)	O(1)#1–Cd(1)–O(2)#1	56.10(10)
N(3)–Cd(1)–O(1)#1	93.17(11)	O(4)#2–Cd(1)–O(2)#1	124.93(12)
N(1)–Cd(1)–O(1)#1	138.38(11)	N(3)–Cd(1)–O(3)#2	84.94(12)
N(3)–Cd(1)–O(4)#2	136.39(12)	N(1)–Cd(1)–O(3)#2	93.09(10)
N(1)–Cd(1)–O(4)#2	89.22(13)	O(1)#1–Cd(1)–O(3)#2	122.41(10)
O(1)#1–Cd(1)–O(4)#2	93.90(10)	O(4)#2–Cd(1)–O(3)#2	55.43(12)
N(3)–Cd(1)–O(2)#1	94.13(12)	O(2)#1–Cd(1)–O(3)#2	178.23(9)
N(1)–Cd(1)–O(2)#1	88.65(10)		

Compound **4**[d]

Cd(1)–N(1)#1	2.253(4)	Cd(1)–O(1)#3	2.287(4)
Cd(1)–N(1)	2.253(4)	Cd(1)–O(2)#2	2.431(4)
Cd(1)–O(1)#2	2.287(4)	Cd(1)–O(2)#3	2.431(4)
N(1)#1–Cd(1)–N(1)	106.5(3)	O(1)#2–Cd(1)–O(2)#2	55.22(13)
N(1)#1–Cd(1)–O(1)#2	96.68(16)	O(1)#3–Cd(1)–O(2)#2	113.36(16)

N(1)–Cd(1)–O(1)#2	92.54(16)	N(1)#1–Cd(1)–O(2)#3	146.95(14)
N(1)#1–Cd(1)–O(1)#3	92.54(15)	N(1)–Cd(1)–O(2)#3	86.33(19)
N(1)–Cd(1)–O(1)#3	96.68(16)	O(1)#2–Cd(1)–O(2)#3	113.36(16)
O(1)#2–Cd(1)–O(1)#3	164.6(3)	O(1)#3–Cd(1)–O(2)#3	55.22(13)
N(1)#1–Cd(1)–O(2)#2	86.33(19)	O(2)#2–Cd(1)–O(2)#3	99.3(2)
N(1)–Cd(1)–O(2)#2	146.95(14)		

Compound **5**[e]

Co(1)–O(2)#1	2.070(3)	Co(1)–N(2)#3	2.080(3)
Co(1)–O(2)#2	2.070(3)	Co(1)–O(1)#1	2.323(3)
Co(1)–N(2)	2.080(3)	Co(1)–O(1)#2	2.323(3)
O(2)#1–Co(1)–O(2)#2	163.4(2)	N(2)–Co(1)–O(1)#1	87.39(12)
O(2)#1–Co(1)–N(2)	95.55(13)	N(2)#3–Co(1)–O(1)#1	151.01(12)
O(2)#2–Co(1)–N(2)	94.18(13)	O(2)#1–Co(1)–O(1)#2	108.02(13)
O(2)#1–Co(1)–N(2)#3	94.18(13)	O(2)#2–Co(1)–O(1)#2	59.17(13)
O(2)#2–Co(1)–N(2)#3	95.55(13)	N(2)–Co(1)–O(1)#2	151.01(12)
N(2)–Co(1)–N(2)#3	107.93(18)	N(2)#3–Co(1)–O(1)#2	87.39(12)
O(2)#1–Co(1)–O(1)#1	59.17(13)	O(1)#1–Co(1)–O(1)#2	90.39(17)
O(2)#2–Co(1)–O(1)#1	108.02(13)		

Compound **6**[f]

Cd(1)–N(3)	2.225(10)	Cd(1)–O(3)	2.311(6)
Cd(1)–O(1)	2.289(5)	Cd(1)–O(2)	2.437(5)
Cd(1)–N(1)	2.300(7)	Cd(1)–O(4)	2.448(7)
N(3)–Cd(1)–O(1)	95.6(3)	N(1)–Cd(1)–O(2)	142.4(2)

N(3)–Cd(1)–N(1)	106.0(3)	O(3)–Cd(1)–O(2)	104.2(2)
O(1)–Cd(1)–N(1)	93.0(2)	N(3)–Cd(1)–O(4)	151.9(3)
N(3)–Cd(1)–O(3)	96.5(3)	O(1)–Cd(1)–O(4)	108.6(3)
O(1)–Cd(1)–O(3)	157.3(2)	N(1)–Cd(1)–O(4)	87.3(3)
N(1)–Cd(1)–O(3)	101.9(2)	O(3)–Cd(1)–O(4)	56.0(2)
N(3)–Cd(1)–O(2)	97.4(3)	O(2)–Cd(1)–O(4)	85.4(3)
O(1)–Cd(1)–O(2)	55.23(19)		

[a]Symmetry transformations used to generate equivalent atoms:

#1 -x-1,y-1,-z #2 x+1,y-1,z #3 -x,y,-z #4 x-1,y+1,z

[b]Symmetry transformations used to generate equivalent atoms:

#1 -x-1,y-1,-z #2 x+1,y-1,z #3 -x,y,-z #4 x-1,y+1,z

[c]Symmetry transformations used to generate equivalent atoms:

#1 x-1/2,-y+3,z #2 -x+1,-y+1,z-1/2 #3 x+1/2,-y+3,z #4 -x+1,-y+1,z+1/2

[d]Symmetry transformations used to generate equivalent atoms:

#1 y,x,-z+1 #2 x-1/2,-y+3/2,-z #3 -y+3/2,x-1/2,z+1 #4 y+1/2,-x+3/2,z-1

[e]Symmetry transformations used to generate equivalent atoms:

#1 -y+1/2,x+1/2,z+1 #2 x+1/2,-y+1/2,-z #3 y,x,-z+1 #4 y-1/2,-x+1/2,z-1

[f]Symmetry transformations used to generate equivalent atoms:

#1 -x+3/2,y+1/2,z #2 -x+5/2,y+0,z-1/2 #3 -x+3/2,y-1/2,z #4 -x+5/2,y+0,z+1/2