Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Zn^{II} and Cd^{II} MOFs based on Amidoisophthalic acid ligand: Synthesis, Structure and Catalytic Application in Transesterification

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Calculation of the yield in the transesterification reaction

The methyl peak of methyl-4-nitrobenzoate (reactant) appears as 3.943 ppm and the methyl of ethyl-4-nitrobenzoate (product) appears at 1.442 ppm.
Total amount of compound: unreacted methyl-4-nitrobenzoate + ethyl-4-nitrobenzoate= 0.090+ 1 = 1.09
Conversion of methyl-4-nitrobenzoate = yield of ethyl-4-nitrobenzoate = 100/1.09 = 91 %

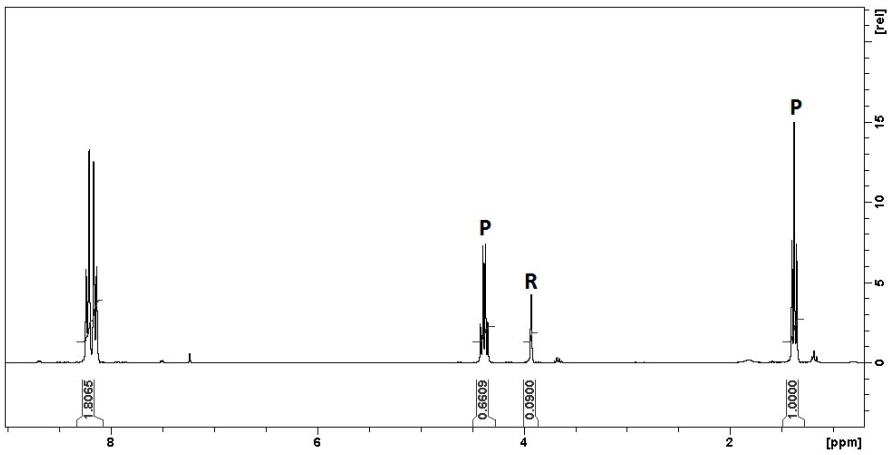
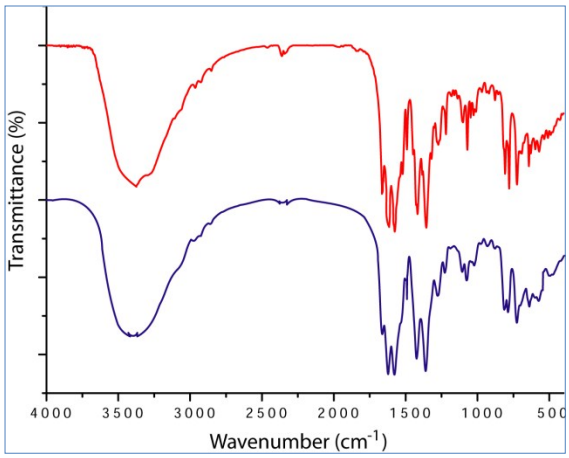
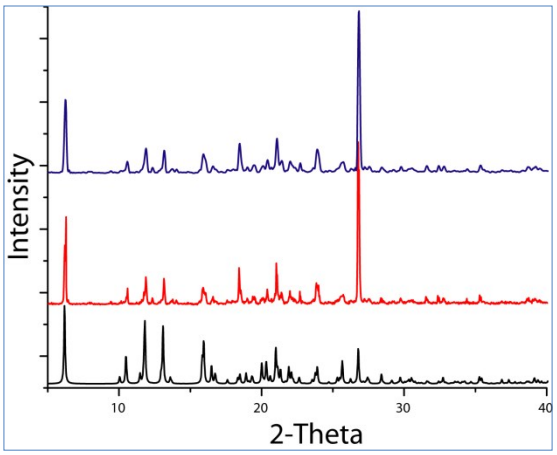


Figure S1. Example of integration in the ^{1}H-NMR spectrum for the determination of transesterification reaction products (Table 1, Entry 6). [P= Product peak (from ethyl group of ethyl-3-nitrobenzoate), R= Unreacted methyl-3-nitrobenzoate (methyl group of methyl-3-benzoate)].

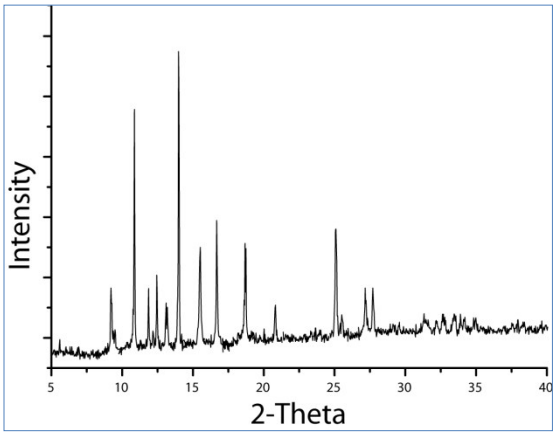


A

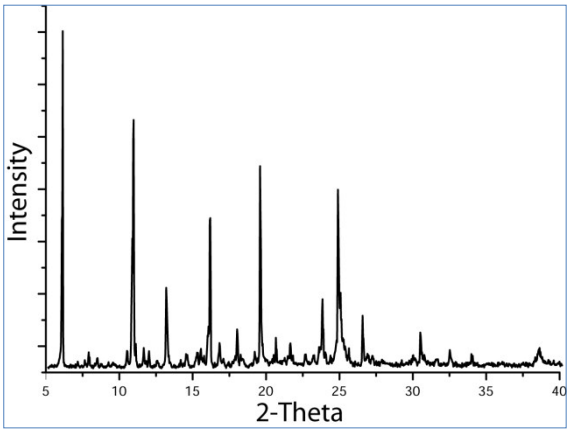


B

Figure S2 (A) FT-IR spectra of **4** before (red line) and after (blue line) the transesterification reaction. (B) Powder XRD curves of **4** (the red and blue curves refer to before and after the catalysis reaction and the black curve is the theoretical one).



A



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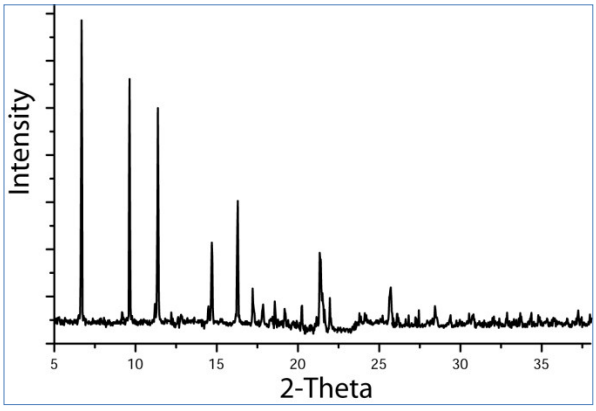

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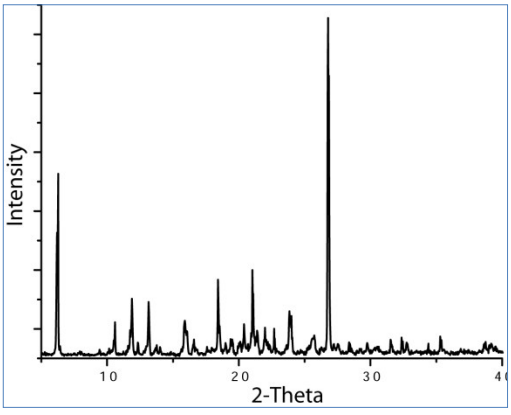

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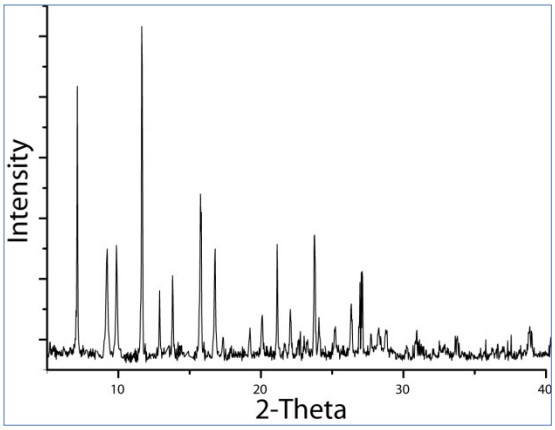
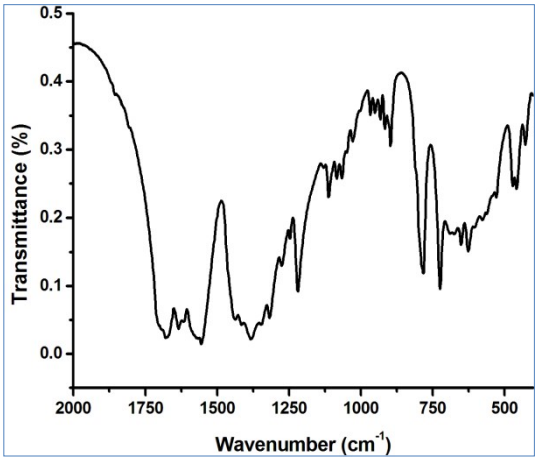
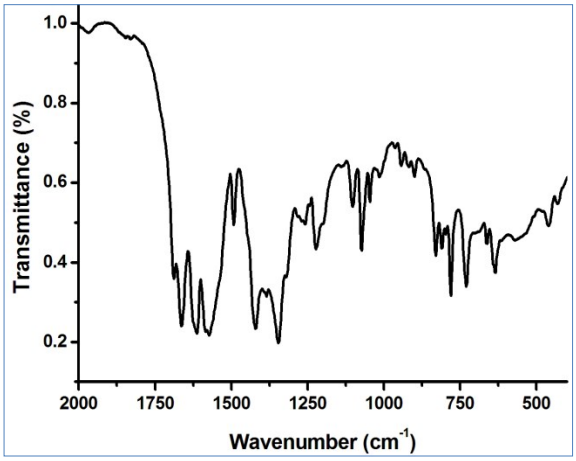


E

Figure S3 Powder XRD spectra of **1** (A), **2** (B), **3** (C), **4** (D) and **5** (E).



A



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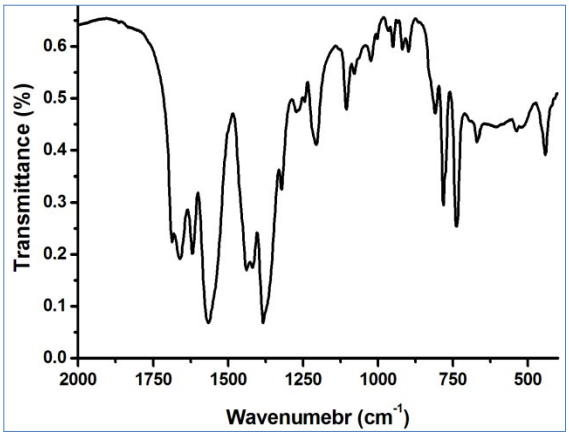

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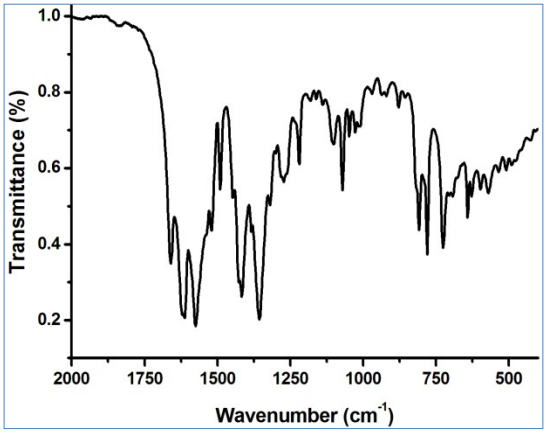
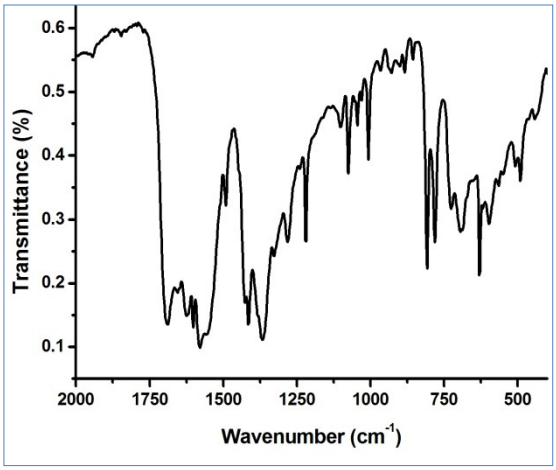


D



E

Figure S4 FT-IR spectra of **1** (A), **2** (B), **3** (C), **4** (D) and **5** (E).

Table S1: Crystal data and structure refinement details for Complex 1-5					
Identification name	**1**	**2**	**3**	**4**	**5**
Formulae	$C_{13}H_{15}N_3O_7Zn$	$C_{48}H_{58}N_8O_{18}Zn_2$	$C_{14}H_{16}CdN_2O_6$	$C_{25}H_{19}N_3O_7Zn$	$C_{27}H_{23}CdN_5O_7$
Mol. wt.	390.65	1165.76	420.69	538.80	641.90
Crystal system	Triclinic	Triclinic	Tetragonal	Monoclinic	Monoclinic
Space group	P -1	P -1	I 4_1cd	C2/c	$P2_1/c$
Temperature /K	296	296	296	296	296
Wavelength /Å	0.71073	0.71073	0.71073	0.71073	0.71073
a /Å	8.7775(9)	11.777(2)	24.9839(7)	15.439(11)	13.0001(6)
b /Å	9.6775(10)	15.197(3)	24.9839(7)	10.758(7)	10.0706(5)
c /Å	9.8961(10)	17.163(3)	10.2525(3)	28.81(2)	20.0881(10)
α/°	81.460(4)	115.964(6)	90	90	90
β/°	69.986(4)	103.286(7)	90	90.73(3)	105.006(2)
γ/°	78.630(4)	90.579(7)	90	90	90
V/ Å^3	771.35(14)	2666.3(9)	6399.6(4)	4785(6)	2540.2(2)
Z	2	2	16	8	4
Density/Mgm^{-3}	1.682	1.452	1.747	1.496	1.678
Abs. Coeff. /mm^{-1}	1.635	0.979	1.396	1.078	0.918
F(000)	400	1212	3360	2208	1296
Refl. collected	11963	52466	35966	26406	51716
Refl. unique	3778	13182	2916	4408	5210
Max. 2θ/°	28.288	28.333	25.363	25.442	26.423
Ranges (h, k, l)	-11<= h <=11 -12<= k <=12 -13<= l <= 13	-15<= h <=15 -20<= k <=20 -22<= l <= 22	-30<= h <=30 -30<= k <=30 -12<= l <= 12	-18<= h <=18 -12<= k <=12 -34<= l <= 34	-16<= h <=16 -12<= k <=12 -25<= l <= 25

Complete to 2θ (%)	98.6	99.1	99.9	99.5	99.7
Refl. with I > 2σ(I)	3142	10717	2839	3267	4528
Data/ Restraints/Parameters	3778/7/233	13182/1/711	2916/2/214	4408/124/380	5210/3/376
Goof (F^2)	1.070	1.085	1.068	1.045	1.123
R1 [I > 2s(I)]	0.0390	0.0396	0.0262	0.0956	0.0346
wR2 [I > 2s(I)]	0.0978	0.0986	0.0628	0.2488	0.0794
R1 [all data]	0.0523	0.0532	0.0271	0.1224	0.0429
wR2 [all data]	0.1046	0.1062	0.0639	0.2761	0.0835

Table S2: Selected bond distances (Å) and angles (°) for compounds 1-5	
Compound 1	Zn1-O4, 1.9713(18); Zn1-O2, 1.9758(17); Zn1-O1, 1.9882(17); Zn1-O6, 2.084(2); Zn1-O7, 2.231(2). <O4-Zn1-O2, 135.49(8); <O4-Zn1-O1, 100.09(8); <O2-Zn1-O1, 123.54(8); <O4-Zn1-O6, 91.91(9); <O2-Zn1-O6, 97.67(8); <O1-Zn1-O6, 87.73(8); <O4-Zn1-O7, 87.01(8); <O2-Zn1-O7, 86.32(8); <O1-Zn1-O7, 87.90(8); <O6-Zn1-O7, 175.24(8).
Compound 2	Zn1-O6, 1.9373(13); Zn1-O1, 1.9446(14); Zn1-N5, 2.0264(15); Zn1-N3, 2.0539(17); Zn2-O4, 1.9871(13); Zn2-O8, 1.9925(14); Zn2-N6, 2.0970(15); Zn2-O11, 2.2007(15); Zn2-N4, 2.2311(17). <O6-Zn1-O1 117.58(6); <O6-Zn1-N5 99.66(6); <O1-Zn1-N5 117.85(6); <O6-Zn1-N3 110.05(7); <O1-Zn1-N3 102.00(7); <N5-Zn1-N3 109.77(7); <O4-Zn2-O8 117.93(6); <O4-Zn2-N6 97.24(6); <O8-Zn2-N6 144.65(6); <O4-Zn2-O11 95.56(6); <O8-Zn2-O11 88.50(6); <N6-Zn2-O11 84.43(6); <O4-Zn2-N4 96.57(6); <O8-Zn2-N4 85.37(7); <N6-Zn2-N4 94.54(6); <O11-Zn2-N4 167.86(6).
Compound 3	Cd1-O3, 2.195(4); Cd1-O4, 2.270(5); Cd1-O1, 2.277(4); Cd1-O2, 2.346(4); Cd1-O6, 2.370(4); Cd1-O1', 2.414(4). <O3-Cd1-O4, 92.58(19); <O3-Cd1-O1, 125.25(16); <O4-Cd1-O1, 89.56(13); <O3-Cd1-O2, 89.65(16); <O4-Cd1-O2, 111.57(17); <O1-Cd1-O2, 139.11(15); <O3-Cd1-O6, 88.7(2); <O4-Cd1-O6, 168.02(18); <O1-Cd1-O6, 80.02(13); <O2-Cd1-O6, 80.34(17); <O3-Cd1-O1, 139.08(15); <O4-Cd1-O1, 83.96(17); <O1-Cd1-O1, 95.55(15); <O2-Cd1-O1, 54.96(14); <O6-Cd1-O1, 102.8(2).
Compound 4	Zn1-N1 2.234(6); Zn1-N2 2.051(7); Zn1-O1 2.206(7); Zn1-O6 1.936(5); Zn1-O3 1.934(7). <O3-Zn1-O6 115.0(3); <O3-Zn1-N2 139.3(2); <O6-Zn1-N2 105.7(2); <O3-Zn1-O1 92.2(3); <O6-Zn1-O1 94.4(2); <N2-Zn1-O1 84.7(3); <O3-Zn1-N1 87.7(3); <O6-Zn1-N1 94.3(2); <N2-Zn1-N1 89.2(3); <O1-Zn1-N1 170.5(3).
Compound 5	Cd1-N2, 2.265(2); Cd1-O3, 2.324(2); Cd1-O5, 2.352(2); Cd1-O6, 2.3711(19); Cd1-O1, 2.551(2); Cd1-O2, 2.649(2). <O1-Cd1-N2 121.66(8); <O1-Cd1-O3 104.82(8); <N2-Cd1-O3 96.11(9); <O1-Cd1-O5 86.04(7); <N2-Cd1-O5 147.27(8); <O3-Cd1-O5 92.51(9); <O1-Cd1-O6 140.04(7); <N2-Cd1-O6 93.10(8); <O3-Cd1-O6 88.80(8); <O5-Cd1-O6 55.50(7); <O1-Cd1-O1 78.84(7); <N2-Cd1-O1 85.16(8);

	<O3-Cd1-O1 174.55(7); <O5-Cd1-O1 83.66(7); <O6-Cd1-O1 85.84(7); <O1-Cd1-O2 52.55(7); <N2-Cd1-O2 83.01(7); <O3-Cd1-O2 75.28(8); <O5-Cd1-O2 129.71(7); <O6-Cd1-O2 163.04(7); <O1-Cd1-O2 110.15(6); <Cd1-O1-Cd1' 101.16(7).

Table S3: Hydrogen bond geometry (Å, °) in compounds 1-5

Compound	D-H···A	D···H (Å)	H···A (Å)	D···A (Å)	<D−H···A(°)	Symmetry
1	N3-H3B···O5	0.86	2.10	2.893(4)	152.9	x, y+1, z-1
	N3-H3A···O3	0.86	2.25	3.019(4)	149.6	-x, -y+1, -z+2
	N2-H2B···O5	0.86	2.06	2.888(4)	162.0	x+1, y, z-1
	N2-H2A···O3	0.86	2.09	2.949(3)	172.3	-x+1, -y, -z+2
	N1-H1···O7	0.86	2.20	3.059(3)	173.0	x, y-1, z
2	N1-H1···O14A	0.86	2.26	3.068(4)	155.6	-x+1, -y+2, -z+1
	N2-H2···O16	0.86	2.09	2.934(2)	165.4	-x+1, -y+2, -z+1
	O11-H12O···O9	0.85	1.89	2.732(2)	168.2	-x+2, -y+2, -z+1
	O16-H16A···O15	0.83	1.87	2.687(3)	168.0	-
	O15-H15B···O3	0.88	1.84	2.717(2)	173.6	-x, -y+1, -z+1
	O15-H15A···O12	0.87	1.94	2.785(3)	163.4	-x+1, -y+1, -z+1
	O17-H17B···O16	0.93	1.82	2.747(3)	173.0	-
	O16-H16B···O2	0.83	1.93	2.716(2)	156.3	-x+1, -y+1, -z+1
	O17-H17O···O1	0.85	1.97	2.821(2)	173.0	-
	O18-H18A···O7	0.91	1.91	2.798(3)	168.0	-
	O18-H18B···O14A	0.81	1.94	2.681(4)	151.7	x, y+1, z-1
	O11-H11O···O14A	0.85	1.98	2.820(3)	167.8	-
	O11-H11O···O14B	0.85	1.95	2.704(5)	146.8	-
3	O5-H5A···O7	0.96	2.05	2.839(11)	138.3	-x+1, -y+1, -z+2
	O5-H5B···O3	0.96	1.83	2.768(8)	164.8	-x, -y+1, -z+2
	C21-H21···O3	0.93	2.61	3.370(8)	139.3	
4	C5-H5···O5	0.93	2.56	3.357(7)	143.5	-x+2, y, z+1/2
	C10-H10A···O2	0.97	2.56	3.528(8)	176.0	-x+2, y, z+1/2
	C3-H3···O5	0.93	2.29	2.886(7)	121.3	-
	C12-H12···O2	0.93	2.50	3.128(11)	124.9	-y+1, x-1/2, z+1/4
5	N4-H5A···O6	0.86	2.20	2.957(4)	146.9	-
	N4-H5B···O2	0.86	2.31	3.071(4)	147.3	x, -y+3/2, z+1/2
	N4-H5B···O3	0.86	2.54	3.204(4)	134.3	-x+1, y+1/2, -z+1/2
	N5-H4A···O8	0.86	2.20	3.044(5)	166.4	-x+2, -y+1, -z+2
	N5-H4B···O5	0.86	2.46	3.215(5)	146.6	-x+1, -y+1, -z+1
	N1-H1N···O8	0.85	2.35	3.145(4)	155.0	x, y, z-1
	C21-H21···O2	0.93	2.50	3.119(4)	124.6	-x+1, -y+1, -z

	C20-H20···O7	0.93	2.57	3.415(4)	151.9	x, y-1, z
	C26-H26···O7	0.93	2.65	3.379(5)	135.8	-x+2, y-1/2, -z+1/2
	C7-H7···O8	0.93	2.56	3.263(4)	132.9	x, y, z-1
	C5-H5···O7	0.93	2.24	2.835(4)	121.5	-
	C27-H27···O1	0.93	2.61	3.539(6)	174.7	x, y, z+1