Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information

Zinc Amidoisophthalate Complexes and their Catalytic Application in Diastereoselective Henry Reaction

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Table S1: Crystal data and structure refinement details for **1-4**

Identification name	**1**	**2**	**3**	**4**
Formulae	$C_{11}H_{17}NO_9Zn$	$C_{11}H_{21}NO_{11}Zn$	$C_{15}H_{13}NO_7Zn$	C15 H17 N O9 Zn
Mol. wt.	372.62	408.66	384.63	420.66
Crystal system	Orthorhombic	Triclinic	Orthorhombic	triclinic
Space group	Pbca	P-1	$P2_12_12_1$	P-1
Temperature /K	296	296	296	296
Wavelength /Å	0.71073	0.71073	0.71073	0.71073
a /Å	12.3453(12)	7.0755(2)	5.2989(5)	8.9796(17)
b /Å	12.0038(12)	11.1714(3)	15.3102(12)	10.1531(16)
c /Å	20.971(2)	12.1991(4)	19.3432(17)	10.6054(18)
α/°	90	73.1520(10)	90	89.721(7)
β/°	90	82.4800(10)	90	77.398(7)
γ/°	90	72.0420(10)	90	71.835(6)
V/ Å^3	3107.7(5)	877.00(5)	1569.3(2)	894.5(3)
Z	8	2	4	2
Density/Mgm^{-3}	1.593	1.548	1.628	1.562
Abs. Coeff. /mm^{-1}	1.624	1.454	1.603	1.421
F(000)	1536	424	784	432
Refl. collected	49680	17801	18056	17485
Refl. unique	3192	4353	3780	3668
Max. 2θ/°	26.406	28.311	28.337	26.390
Rint	0.0430	0.0280	0.0219	0.0575
Ranges (h, k, l)	-15 <= h <=15 -15 <= k <=15 -26 <= l <= 26	-9 <= h <=9 -14 <= k <=14 -16 <= l <= 16	-7 <= h <= 7 -19<= k <=19 -25 <= l <=25	-11 <= h <= 11 -12<= k <=12 -13 <= l <=13
Complete to 2θ (%)	99.9	99.8	97.5	99.8

Refl. with I > 2σ(I)	2665	3816	3691	2853
Data/ Restraints/Parameters	3192/8 / 224	4353/13/ 260	3780/ 0/ 220	3668/8/263
Goof (F^2)	1.056	1.077	1.063	1.056
R1 [I > 2s(I)]	0.0422	0.0471	0.0337	0.0405
wR2 [I > 2s(I)]	0.1108	0.1211	0.0883	0.0940
R1 [all data]	0.0518	0.0539	0.0343	0.0619
wR2 [all data]	0.1186	0.1267	0.0893	0.1030

Table S2: Hydrogen bond geometry (Å, °) in compounds **1-4**

Compound	D-H---A	D-H (Å)	H···A (Å)	D···A (Å)	<D−H···A(°)	Symmetry
1	N1-H1N····O2	0.86	2.15	2.987(3)	164.0	-x+1/2, y-1/2, z
	O9-H9A····O4	0.86	1.79	2.647(3)	171.0	x, y-1, z
	O9-H9B····O1	0.85	2.02	2.794(3)	150.0	-x+1, -y+1, -z+1
	O6-H6B····O9	0.87	2.12	2.924(4)	153.0	-x+1, -y+1, -z+1
	O6-H6A····O3	0.87	2.09	2.943(4)	166.0	x, -y+5/2, z+1/2
	O8-H8A····O4	0.86	2.05	2.905(3)	172.0	x, -y+5/2, z+1/2
	O8-H8B····O5	0.88	2.35	3.203(4)	163.0	-x+1, -y+2, -z+1
	O7-H7B····O3	0.87	2.53	3.330(4)	155.0	x-1/2, -y+5/2, -z+1
	O7-H7B····O4	0.87	2.43	3.136(4)	139.0	x-1/2, -y+5/2, -z+1
	O7-H7A····O9	0.86	2.28	3.131(4)	171.0	-x+1/2, -y+1, z+1/2
	C8-H8····O2	0.93	2.65	3.402(3)	138.4	-x+1/2, y-1/2, z
	C6-H6····O5	0.93	2.26	2.877(3)	122.8	-
2	N1-H1N····O11	0.90	2.13	3.029(4)	174.8	x, y, z-1
	O7-H7A····O3	0.94	2.08	3.012(3)	170.0	x, y+1, z
	O7-H7B····O1	0.95	2.11	2.968(3)	150.0	-x, -y+1, -z
	O6-H6A····O3	0.94	2.03	2.956(3)	172.0	x-1, y+1, z
	O6-H6B····O1	0.95	2.04	2.902(3)	151.0	-x, -y+1, -z
	O9-H9A····O4	0.89	1.91	2.781(3)	166.0	-x+1, -y, -z+1
	O9-H9B····O3	0.87	1.97	2.768(3)	151.0	x, y+1, z
	O10-H10o····O4	0.88	2.03	2.841(4)	153.0	-x+1, -y, -z+1
	O10-H9o····O10	0.86	2.43	2.917(7)	116.0	-x+2, -y, -z+1
	O8-H8A····O9	0.93	2.07	2.980(5)	167.0	-x, -y+1, -z+1
	O8-H8B····O9	0.94	2.00	2.942(4)	177.0	-
	O11-H11o····O4	0.93	2.12	3.043(5)	169.1	-x+1, -y, -z+1
	C6-H6····O5	0.93	2.29	2.889(3)	121.5	-
3	O6-H6B····O7	0.97	1.97	2.932(4)	174.4	x-1/2, -y+1/2, -z
	O5-H5A····O4	0.95	2.02	2.944(4)	162.8	x-1/2, -y+1/2, -z
	O6-H6A····O2	0.91	2.30	2.917(4)	125.0	-
	O5-H5B····O4	0.94	1.96	2.870(4)	162.1	x-1, y, z
	C6-H6····O7	0.93	2.35	2.916(4)	118.7	-
4	O6-H6A····O9	0.90	2.15(2)	3.041(4)	169.0	-x+1, -y+1, -z+1
	O6-H6B····O2	0.90	2.09(2)	2.970(4)	164.0	-x+2, -y+1, -z+1
	O7-H7A····O1	0.90	2.16(3)	3.014(3)	159.0	-x+1, -y+1, -z+1
	O7-H7B····O9	0.89	2.17(2)	3.056(4)	177.0	x+1, y, z
	N1-H1N····O8	0.80	2.16(4)	2.950(4)	170.0	-x+1, -y+1, -z+1
	O9-H9B····O5	0.89	1.91(2)	2.786(4)	169.0	x, y-1, z-1

	O8-H8B····O3	0.87	1.93(2)	2.784(4)	165.0	x, y-1, z
	O8-H8A····O3	0.88	1.96(2)	2.848(4)	174.0	-x+2, -y+1, -z+1
	O9-H9A····O8	0.88	2.36(2)	3.190(5)	158.0	x-1, y, z

Table S3: Selected bond distances (Å) and angles (°) for compounds **1-4**

1					
	Bond distances		Bond angles		Bond angles
Zn1-O1	2.0008(19)	<O1-Zn1-O7	119.09(13)	<O7-Zn1-O6	105.30(13)
Zn1-O7	2.008(3)	<O1-Zn1-O8	104.48(11)	<O8-Zn1-O6	108.80(12)
Zn1-O8	2.017(3)	<O7-Zn1-O8	116.52(13)		
Zn1-O6	2.026(3)	<O1-Zn1-O6	101.33(10)		
2					
Zn1-O2	1.9680(18)	<O2-Zn1-O6	110.97(9)	<O6-Zn1-O8	112.18(11)
Zn1-O6	2.009(2)	<O2-Zn1-O7	110.97(10)	<O7-Zn1-O8	110.73(11)
Zn1-O7	2.011(2)	<O6-Zn1-O7	110.43(10)		
Zn1-O8	2.014(3)	<O2-Zn1-O8	101.27(11)		
3					
Zn1-O3	1.958(2)	<O3-Zn1-O1	97.86(11)	<O1-Zn1-O5	105.90(13)
Zn1-O1	1.969(2)	<O3-Zn1-O6	115.88(13)	<O6-Zn1-O5	113.31(12)
Zn1-O6	2.006(3)	<O1-Zn1-O6	108.49(11)		
Zn1-O5	2.018(3)	<O3-Zn1-O5	113.58(13)		
4					
Zn1-O1	1.9929(19)	<O1-Zn1-O6	110.90(11)	<O6-Zn1-O7	123.51(12)
Zn1-O6	2.008(3)	<O1-Zn1-O4	98.19(8)	<O4-Zn1-O7	106.03(10)
Zn1-O4	2.014(2)	<O6-Zn1-O4	109.78(11)		
Zn1-O7	2.016(3)	<O1-Zn1-O7	105.39(10)		

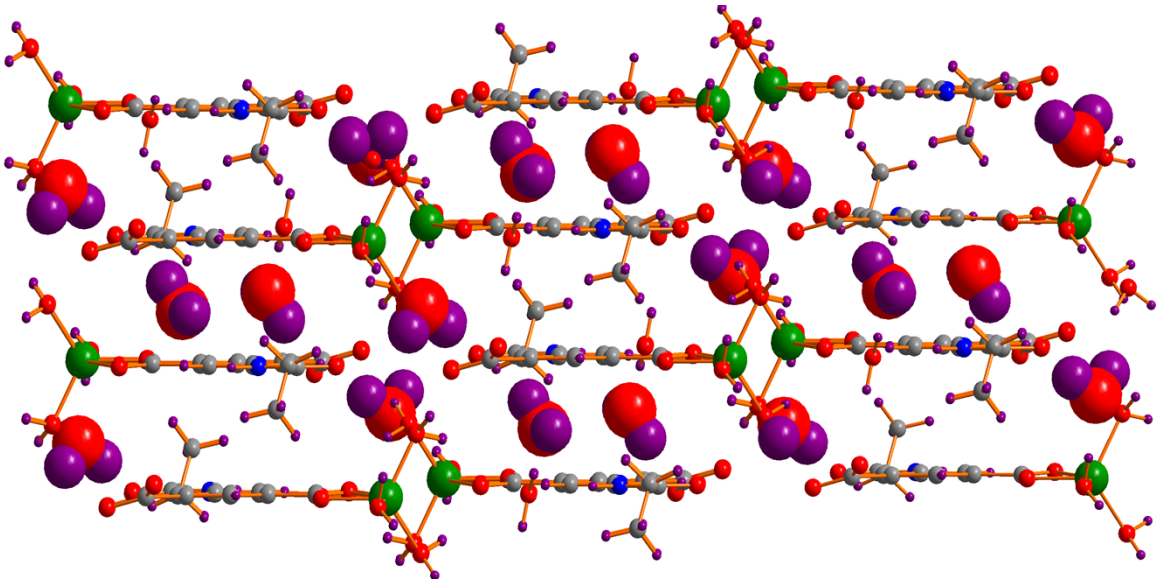
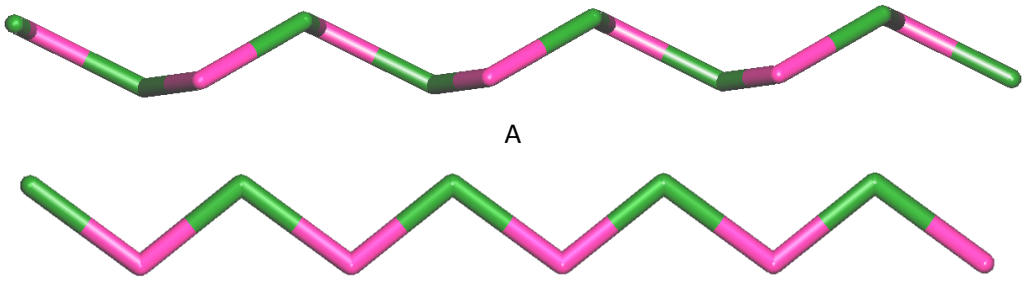


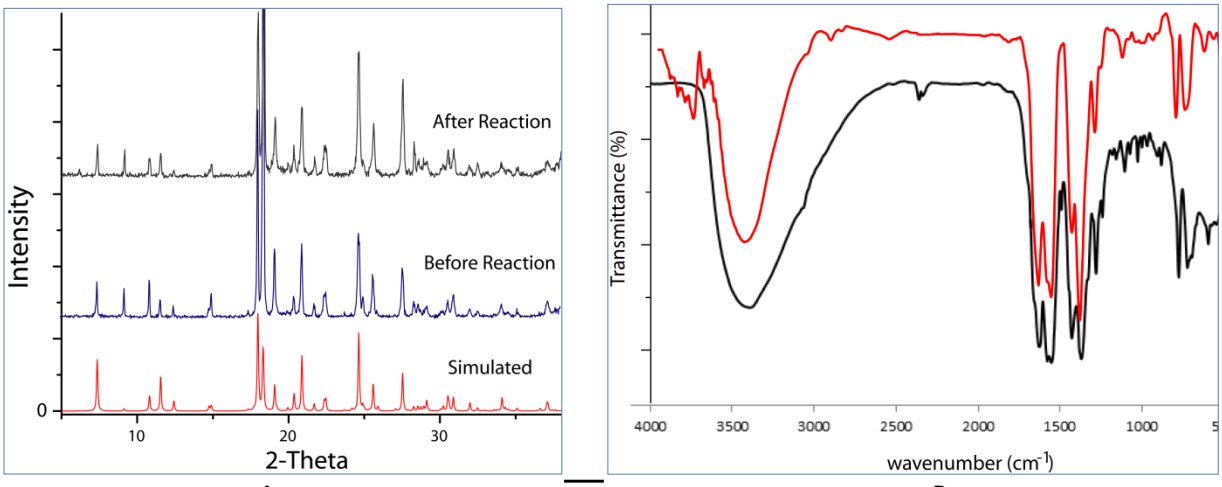
Figure S1 Packing diagram complex **2** (water molecules are represented in spacefill model).



A

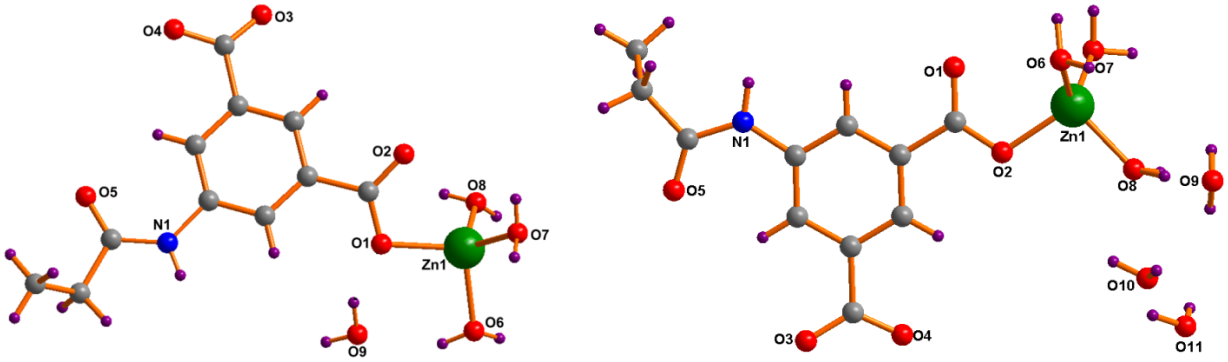
B

Figure S2 Node-and-linker-type descriptions of **3** (A) and **4** (B); the metal nodes are represented in green and the linkers in pink color.



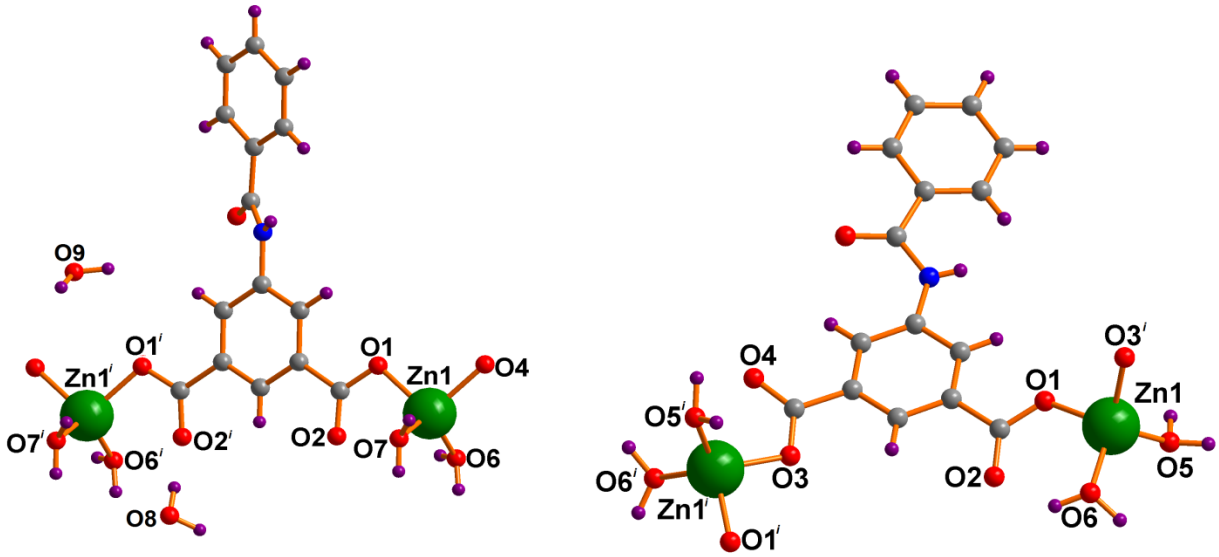
A B

Figure S3 A) Powder XRD curves of **3** before (blue) and after (black) the catalysis reaction (red curve was obtained from the CIF). B) FT-IR spectra of **3** before (in black) and after (in red) the Henry reaction.



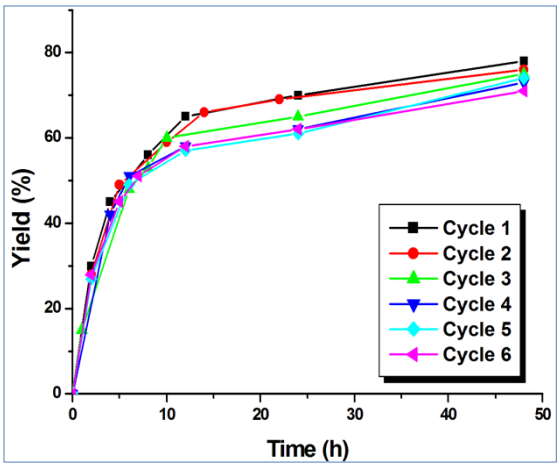
A B

Figure S4 Crystal structures of **1** (A) and **2** (B) with partial atom labelling scheme.

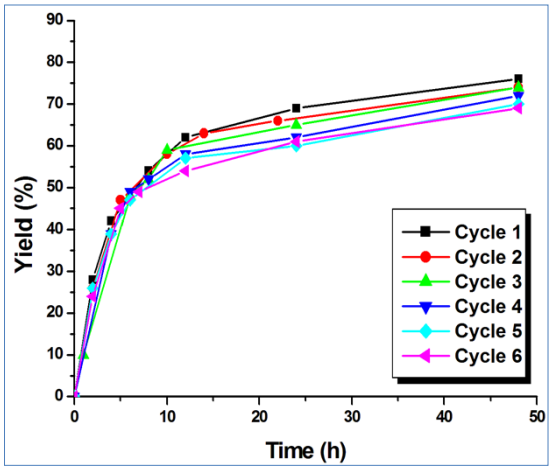


A B

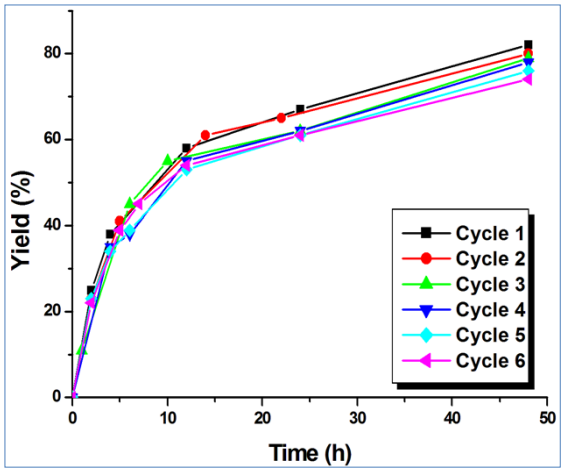
Figure S5 A) Asymmetric unit of **3** with partial atom labelling scheme. B) Asymmetric unit of **4** with partial atom labelling scheme.



A

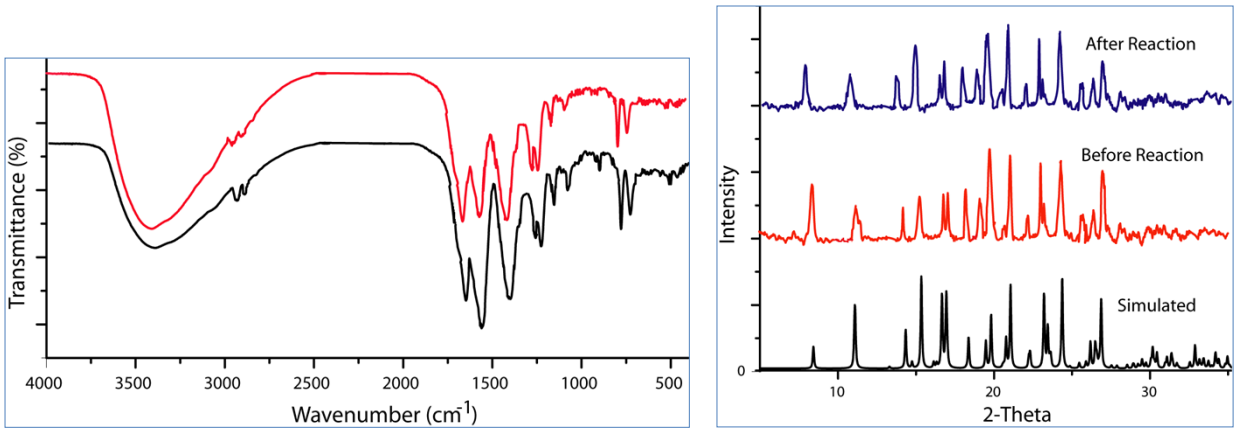


B



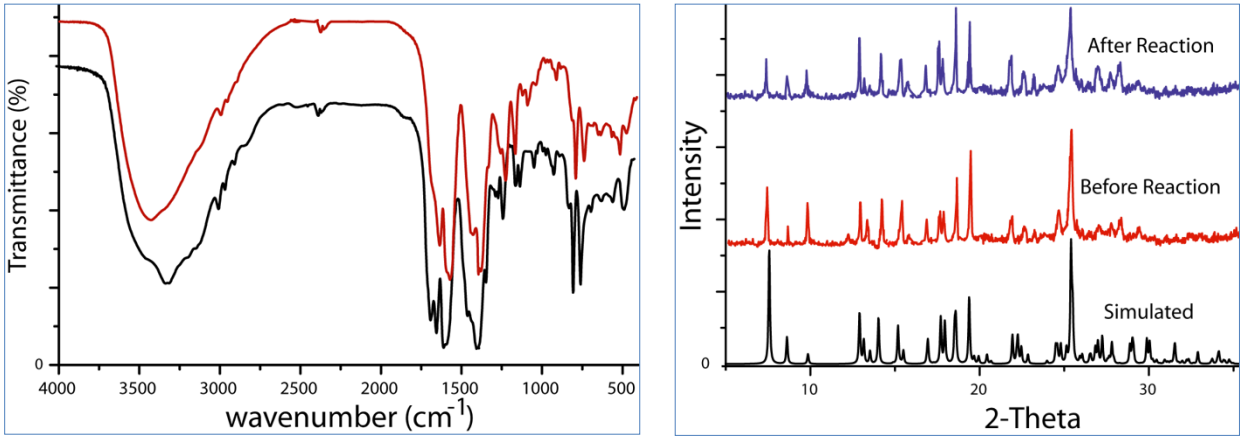
C

Figure S6 Kinetic profiles in six consecutive reaction cycles employing **1** (A), **2** (B) and **4** (C) as catalysts.



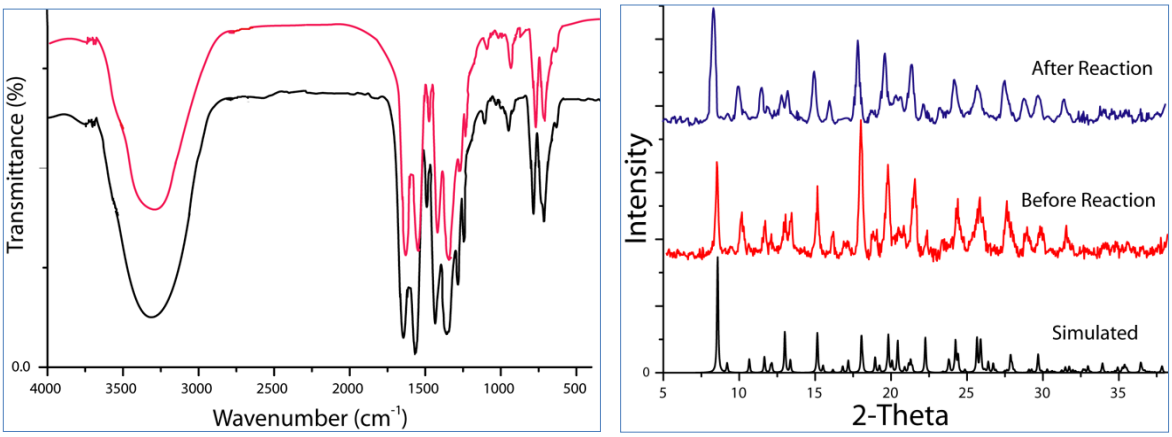
A B

Figure S7 A) FT-IR spectra of **1** before (in black) and after (in red) the Henry reaction. B) Powder XRD curves of **1** before (red) and after (blue) the catalysis reaction (black curve was obtained from the CIF).



A B

Figure S8 A) FT-IR spectra of **2** before (in black) and after (in red) the Henry reaction. B) Powder XRD curves of **2** before (red) and after (blue) the catalysis reaction (black curve was obtained from the CIF).



A B

Figure S9 A) FT-IR spectra of **4** before (in black) and after (in red) the Henry reaction. B) Powder XRD curves of **4** before (red) and after (blue) the catalysis reaction (black curve was obtained from the CIF).