catalysts

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Supplementary Information

1D Zn(II) Coordination Polymers as Effective Heterogeneous Catalysts in Microwave-Assisted Single-Pot Deacetalization-Knoevenagel Tandem Reactions in Solvent-Free Conditions

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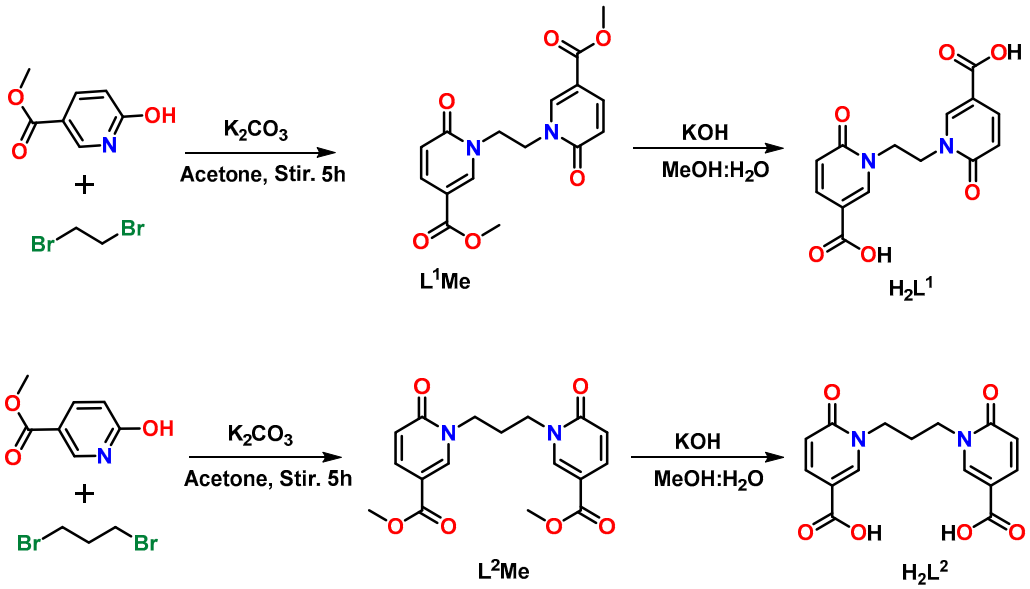

Scheme S1: Synthetic scheme of H_2L^1 and H_2L^2.

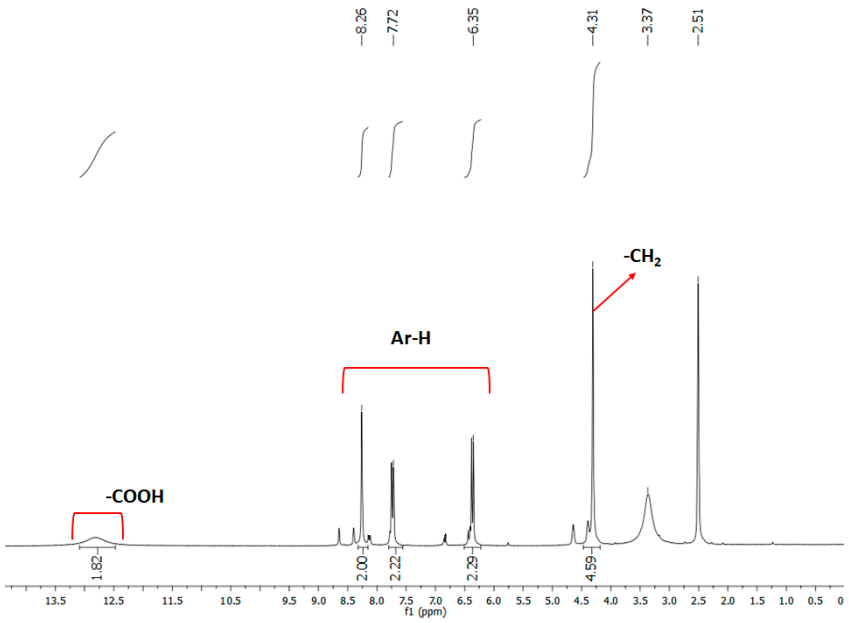

Figure S1. ^{1}H-NMR spectrum of H_2L^1 recorded in DMSO-d_6.

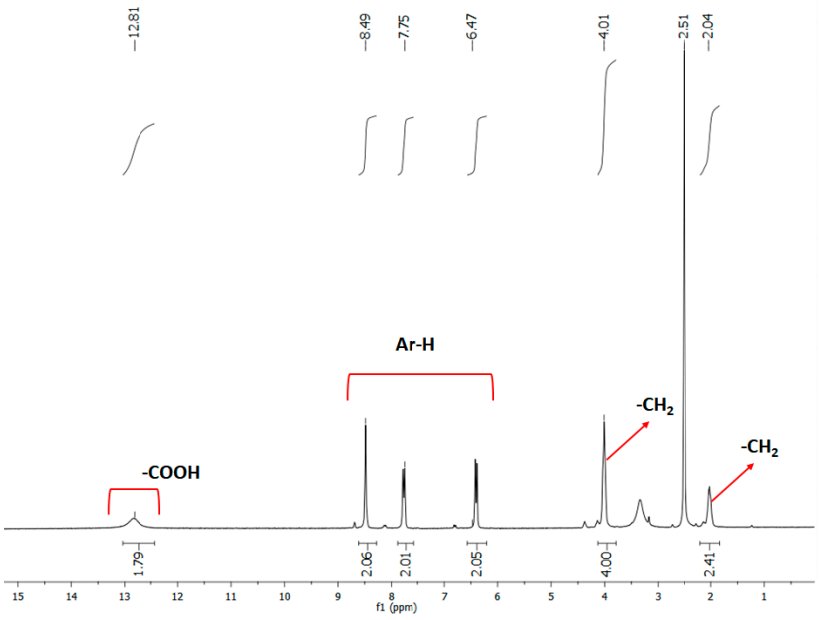

Figure S2. ^{1}H-NMR spectrum of **H$_2$L^2** recorded in DMSO-*d*$_6$.

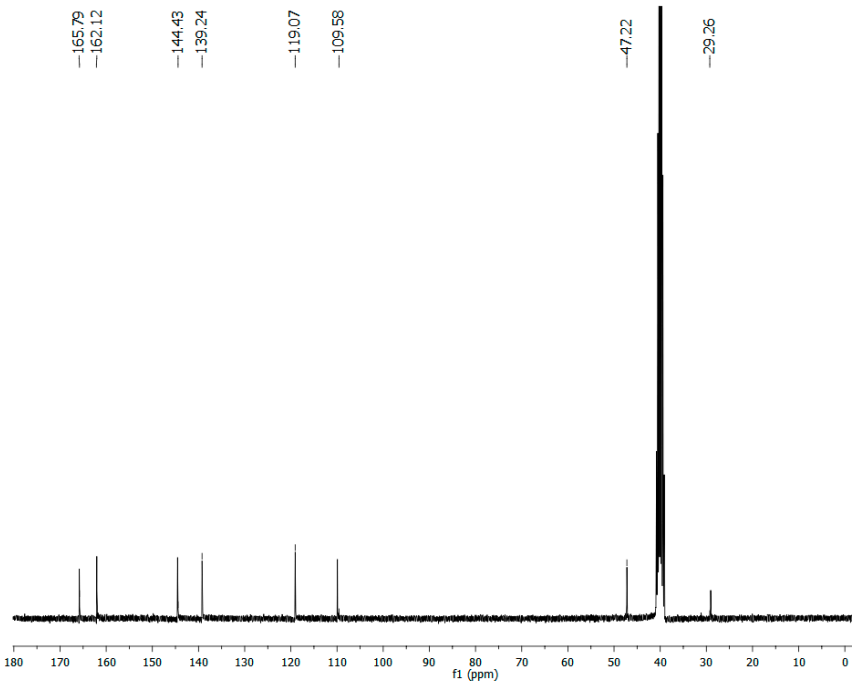

Figure S3. ^{13}C-NMR spectrum of **H$_2$L^1** recorded in DMSO-*d*$_6$.

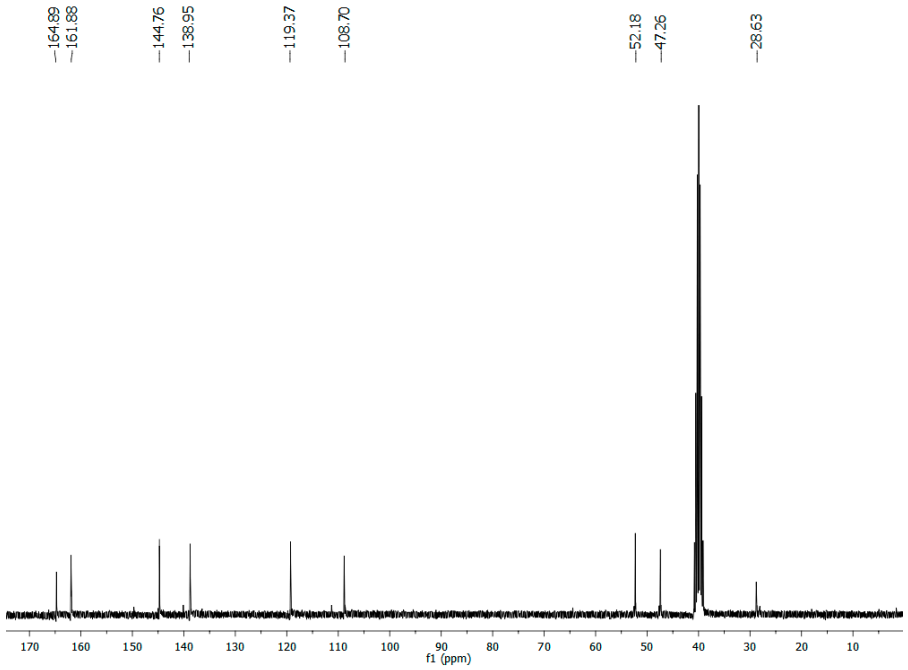

Figure S4. ^{13}C-NMR spectrum of **H$_2$L^2** recorded in DMSO-*d*$_6$.

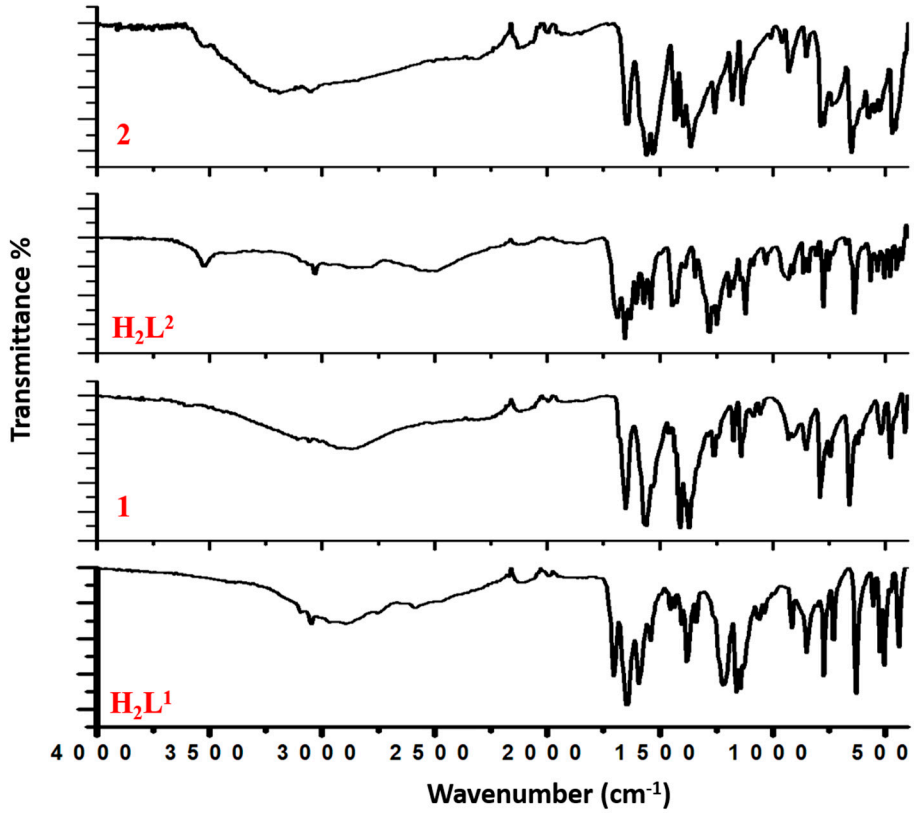

Figure S5. IR spectra of **H$_2$L^1**, **H$_2$L^2** and CPs **1** and **2**.

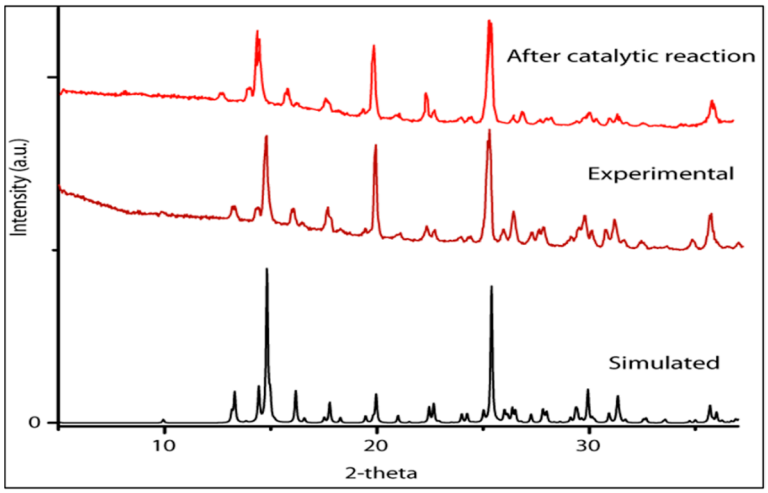

Figure S6: Simulated and experimental PXRD of **1**.

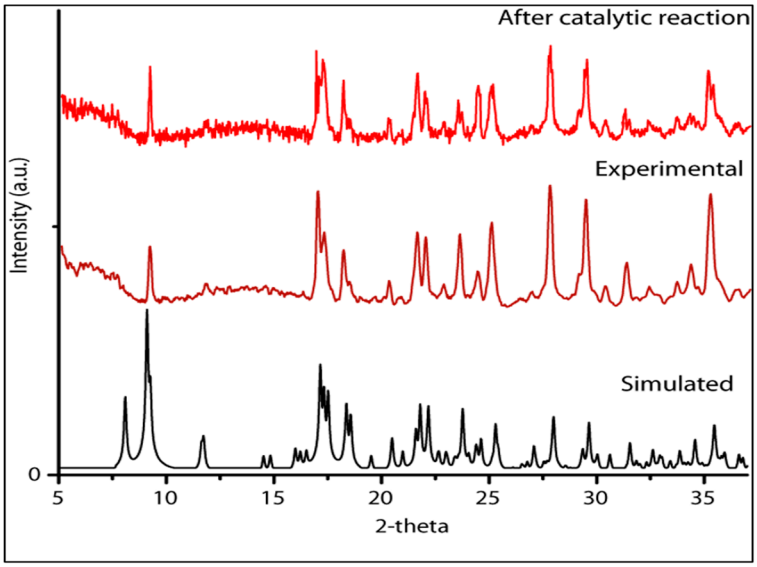

Figure S7. Simulated and experimental PXRD of **2**.

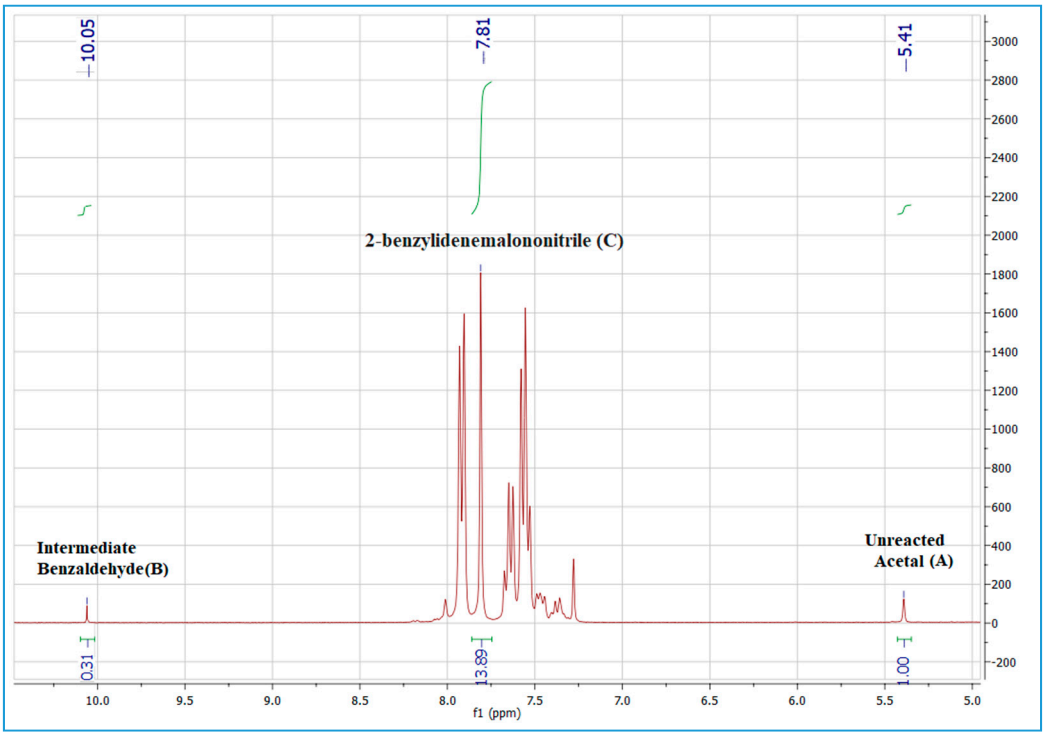

Figure S8. Example of integration in the ^{1}H-NMR spectrum for the determination of the product yield in the one-pot tandem deacetalization–Knoevenagel condensation reactions catalysed by **1** [Table 1, entry 1].

Table S1. Crystal data and structure refinement details for CPs **1** and **2.**

Identification name	**1**	**2**
Formulae	$C_{14}H_{20}N_2O_{11}Zn$	$C_{15}H_{16}N_2O_8Zn$
Mol. wt.	457.69	417.67
Crystal system	Triclinic	Triclinic
Space group	P-1	P-1
Temperature /K	296	296
Wavelength /Å	0.71073	0.71073
a /*Å*	7.0313(19)	8.2951(18)
b /*Å*	7.473(2)	11.330(3)
c /*Å*	18.174(5)	12.174(2)
α/°	78.392(5)	110.907(8)
β/°	82.322(7)	97.686(7)
γ/°	65.624(6)	108.744(8)
V/ Å^3	850.6(4)	971.4(4)
Z	2	2
Density/Mgm^{-3}	1.787	1.428
Abs. Coeff. /mm^{-1}	1.512	1.306
F(000)	472	428
Refl. collected	23257	3606
Refl. unique	3117	3606
Max. 2θ/°	25.242	25.392
Ranges (h, k, l)	−8 <= h <= 8 −8 <= k < =8 −21 <= l <= 21	−10 <= h <= 10 −13 <= k <= 13 −13 <= l <= 14
Complete to 2θ (%)	99.9	99.4
Refl. with I > 2σ(I)	2518	2455
Data/Restraints/Parameters	3117/74/213	3606/0/236
Goof (F^2)	1.161	1.004
R1 [I > 2s(I)]	0.0952	0.0959
wR2 [I > 2s(I)]	0.2903	0.2296
R1 [all data]	0.1157	0.1332
wR2 [all data]	0.3069	0.2568

Table S2. Hydrogen bond geometry (Å, °) in **1** and **2**.

Compound	D-H···A	D···H (Å)	H···A (Å)	D···A (Å)	<D–H···A(°)
1	O7A-H7A1···O4	0.95	2.11	2.827(17)	131
	O7A-H7A2···O20A	0.95	1.75	2.58(3)	143
	O8A-H8A2···O20A	0.95	2.44	3.36(4)	160
	O9-H9A···O6	0.95	2.08	2.840(14)	136
	O9-H9B···O6	0.95	2.03	2.907(13)	152
	O10-H10A···O6	0.95	1.93	2.864(14)	166
	O10-H10B···O5	0.95	2.00	2.633(13)	123
	O20A-H20A···O8A	1.0(3)	1.9(3)	2.88(3)	165
	C6-H6···O20A	0.95	2.41	3.36(2)	173
	C7-H7A···O2	0.99	2.53	3.144(16)	120
	C11-H11···O2	0.95	2.35	3.154(15)	142
2	O(7)-H(6O)···O(2)	0.89	1.89	2.779(9)	179
	O(7)-H(7O)···O(3)	0.89	1.72	2.615(9)	178
	O(8)-H(8O)···O(4)	0.90	1.88	2.782(8)	179
	O(8)-H(9O)···O(6)	0.90	1.72	2.620(10)	179
	C(6)-H(6)···O(7)	0.93	2.59	3.351(10)	140
	C(9)-H(9B)···O(3)	0.97	2.35	3.160(12)	140
	C(15)-H(15) ···O(8)	0.93	2.56	3.348(11)	143

Table S3. Selected bond distances (Å) and angles (°) for **1** and **2**.

1	Zn1-O1 2.022(9), Zn1-O7A 2.074(13), Zn1-O7B 2.146(18), Zn1-O8A 2.143(14), Zn1-O8B 2.163(17), Zn2-O3 2.073(8), Zn2-O10 2.063(8), Zn2-O9 2.153(8). <O1-Zn1-O1 180.0(5), <O1-Zn1-O7A 81.5(5), <O1-Zn1-O7A 98.5(5) , <O7A-Zn1-O7A 180.0, <O1-Zn1-O8A 88.5(5), <O1-Zn1-O8A 91.5(5), <O7A-Zn1-O8A 83.7(5), <O7A-Zn1-O8A 96.3(5), <O8A-Zn1-O8A 180.0, <O1-Zn1-O7B 85.5(6), <O1-Zn1-O7B 94.5(6), <O7B-Zn1-O7B 180.0, <O1-Zn1-O8B 91.1(5), <O1-Zn1-O8B 88.9(5), <O7B-Zn1-O8B 90.7(7), <O7B-Zn1-O8B 89.3(7), <O8B-Zn1-O8B 180.0(8), <O10-Zn2-O10 180.0, <O10-Zn2-O3 90.1(4), <O10-Zn2-O3 89.9(4), <O10-Zn2-O3 90.1(4), <O3-Zn2-O3 180.0, <O10-Zn2-O9 89.7(3), <O10-Zn2-O9 90.3(3), <O3-Zn2-O9 90.8(3), <O3-Zn2-O9 89.2(3), <O9-Zn2-O9 180.0.
2	Zn1-O1 1.961(5), Zn1-O5 1.960(6), Zn1-O8 2.014(6), Zn1-O7 2.020(6). <O1-Zn1-O5 138.1(3), <O1-Zn1-O8 99.8(2), <O5-Zn1-O8 107.5(2), <O1-Zn1-O7 105.9(2), <O5-Zn1-O7 100.0(2), <O8-Zn1-O7 100.1(2).