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

Supporting Information

Designing and Construction of Polyaromatic Group Containing Cd(II)-based Coordination Polymers for Solvent-free Strecker-type Cyanation of Acetals

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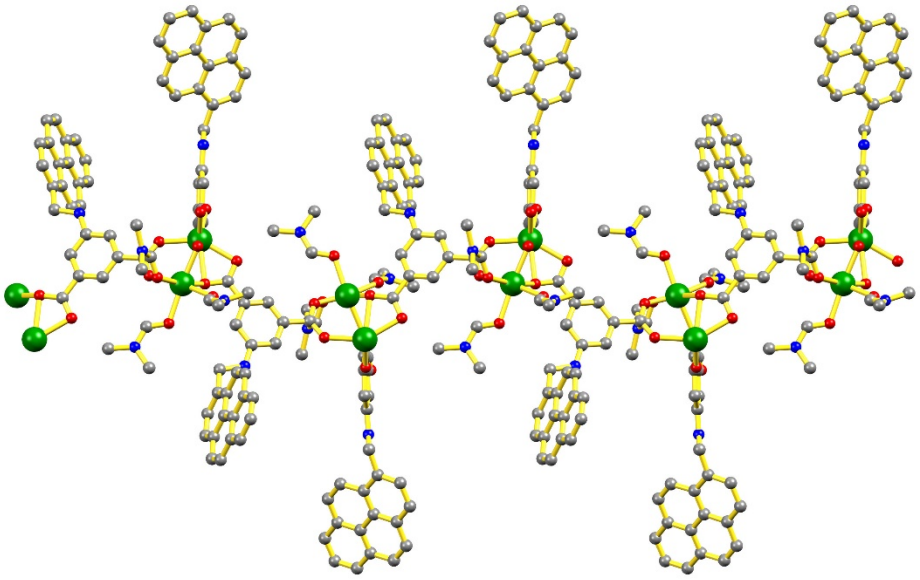


Figure S1 View of framework **2** from *a*-axis.

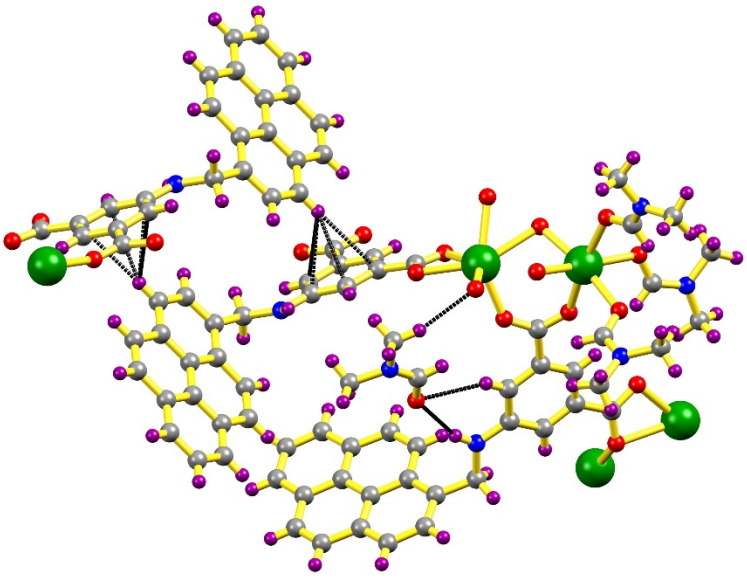
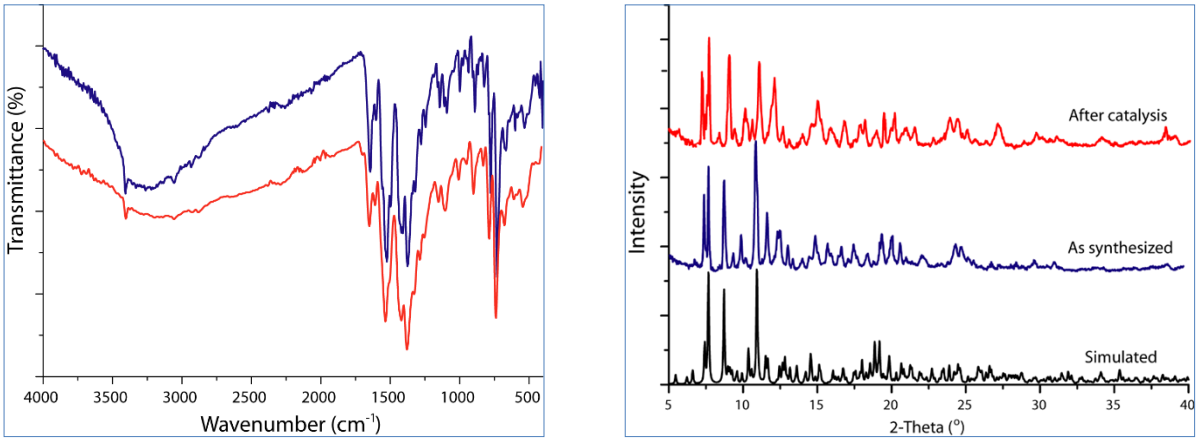
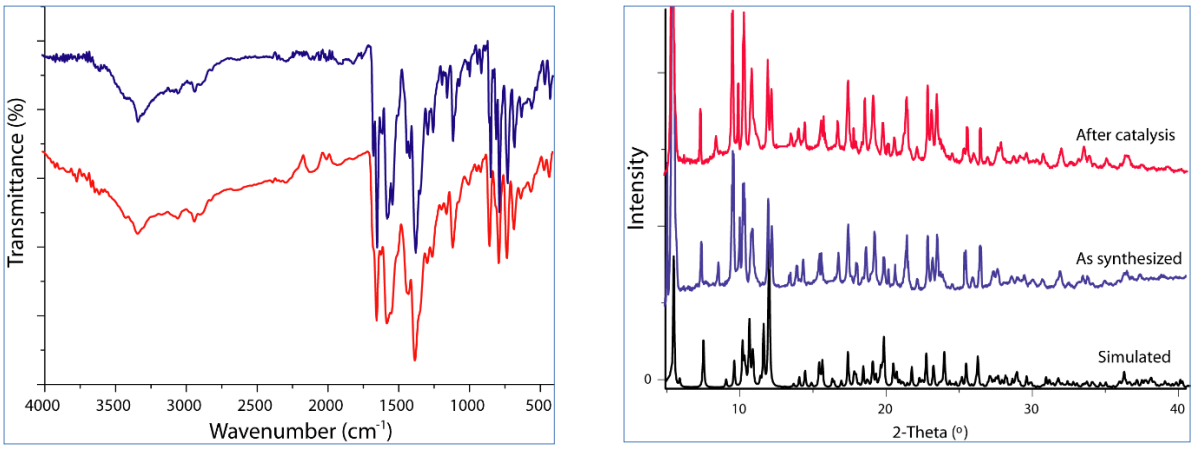


Figure S2 C-H····π, C-H····O and N-H····O interactions present in the CP **2**.



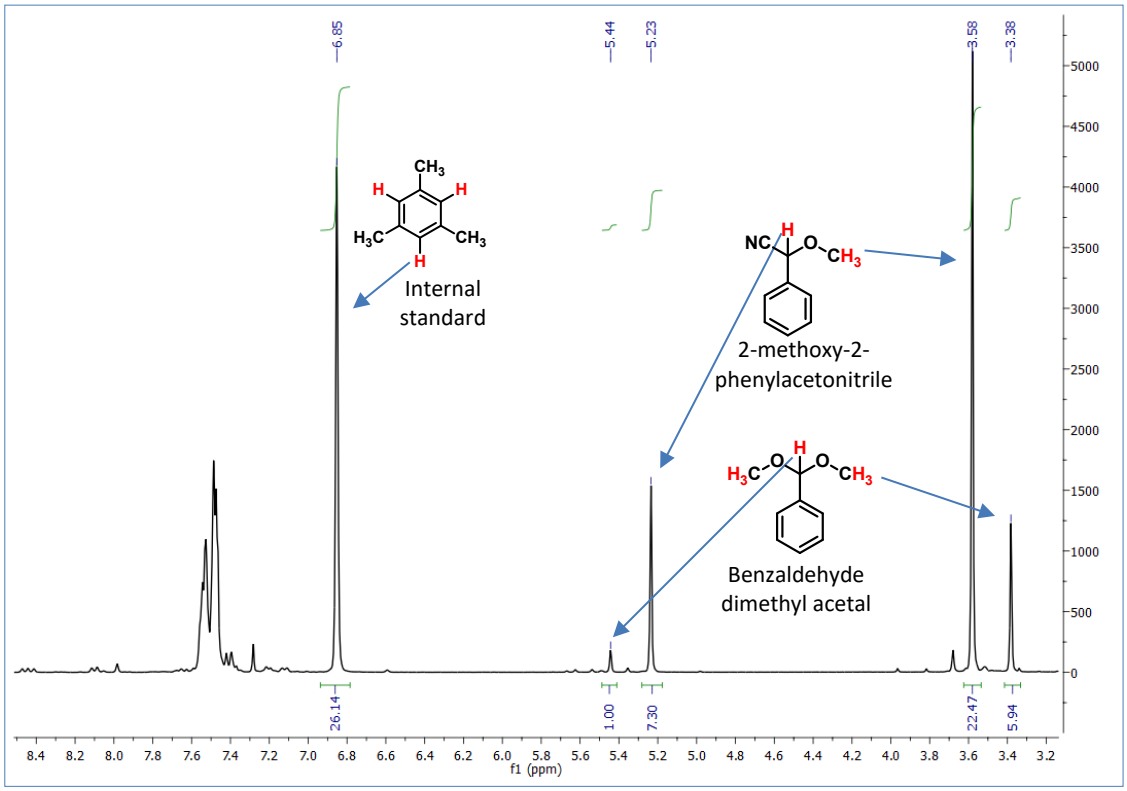
A B

Figure S3 (A) FT-IR spectra of CP **1** before (in blue) and after the cyanation reaction (in red). (B) Powder XRD diffractograms of CP **1** simulated (in black), as synthesized (in blue) and after the cyanation reactions (in red).

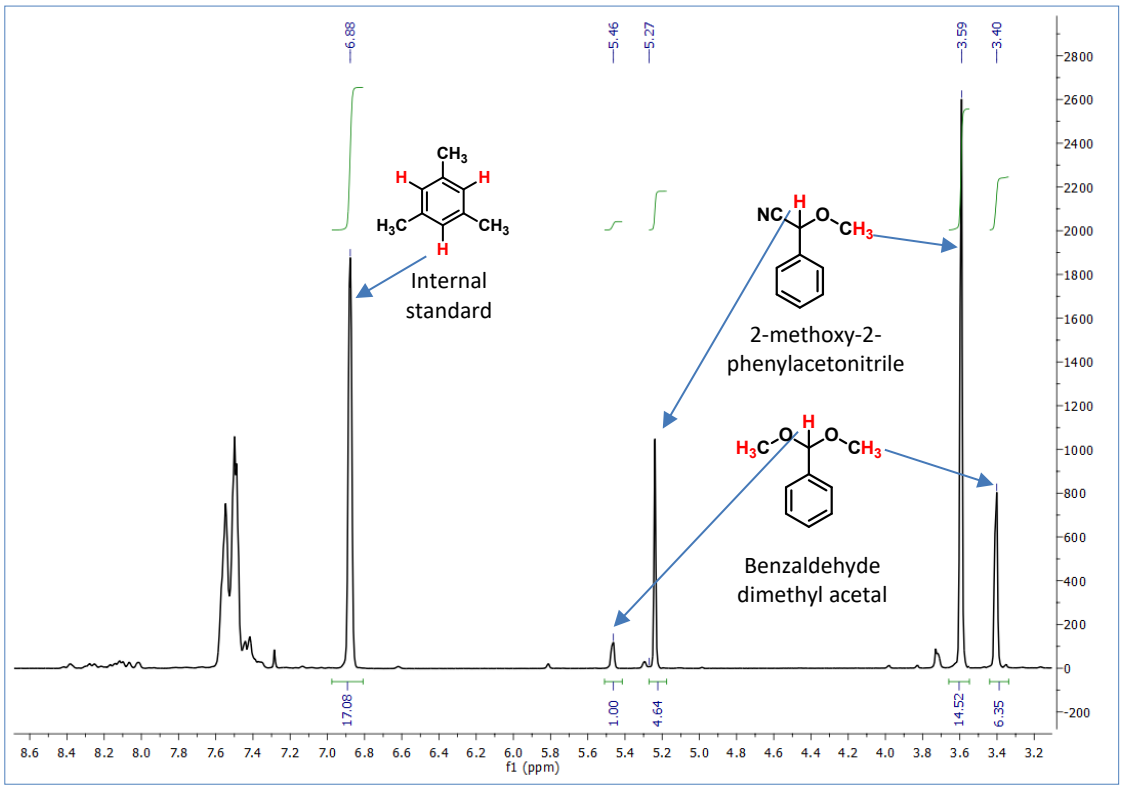


A B

Figure S4 (A) FT-IR spectra of CP **2** before (in blue) and after the cyanation reaction (in red). (B) Powder XRD diffractograms of CP **2** simulated (in black), as synthesized (in blue) and after the cyanation reactions (in red).



A



B

Figure S5 Example of integration in the ^{1}H-NMR spectrum for the determination of the product yield in the cyanation of acetals catalysed by CP **1** (A) and CP **2** (B) under solvent free condition [Table 1, entries 1 and 2].

Reaction yield calculation details from NMR:

In order to calculate the % of yield from H NMR spectroscopy, at first, the molar amount of product (P) was calculated from the molar amount of internal standard (IS) and the molar ratio, where the following formula has been utilized to carry out all the calculations.

The molar ratio of the compound, $r_{P/IS}$ = (integral$_{P/NA}$)/(integral$_{IS/NIS}$) where N = number of nuclei present for the corresponding peaks.

The molar amount of product (P), $n_P = n_{IS} \times r_{P/IS}$

The NMR yield (in %) = (n_P x 100)/(theoretical yield of analyte)

For CP 1: $r_{P/IS}$ = (7.30/1)/(26.14/3) = 0.84

The molar amount of internal standard (IS), n_{IS} : 1.15 mmol

The molar amount of product (P),), $n_P = n_{IS} \times r_{P/IS}$ = 1.15 X 0.84 = 0.966 mmol

The NMR yield (in %) = (n_P x 100)/(theoretical yield of analyte) = (0.966X 100)/ 1.0 = 96.6 %

For CP 2: $r_{P/IS}$ = (4.64/1)/(17.08/3) = 0.82

The molar amount of internal standard (IS), n_{IS} : 1.15 mmol

The molar amount of product (P),), $n_P = n_{IS} \times r_{P/IS}$ = 1.15 X 0.82 = 0.943 mmol

The NMR yield (in %) = (n_P x 100)/(theoretical yield of analyte) = (0.943X 100)/ 1.0 = 94.3 %

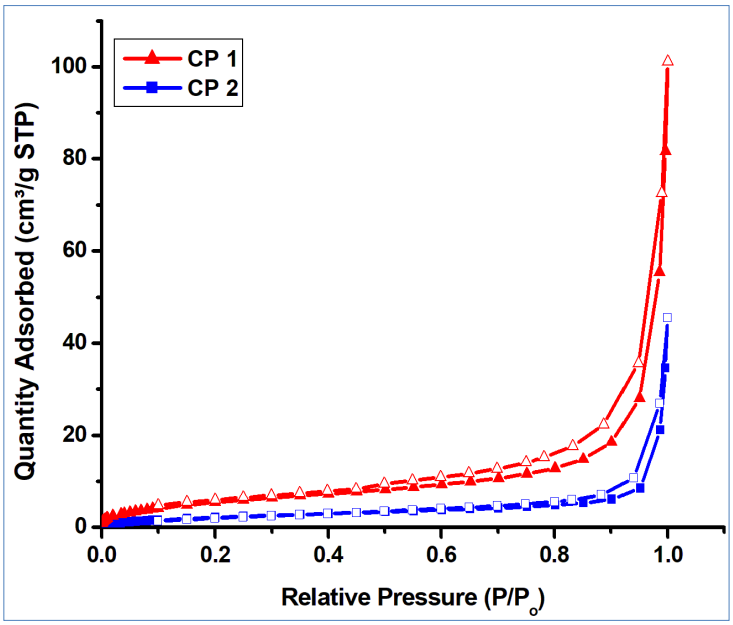


Figure S6 N_2 adsorption isotherms of CPs **1** and **2** after recovered from catalytic reactions [solid symbols represent the adsorption curves and the empty symbols indicate the desorption curves].

Table S1: Crystal data and structure refinement details for compounds 1-2		
Identification name	**1**	**2**
Formulae	$C_{119}H_{122}Cd_4N_{13}O_{25}$	C65 H65 Cd2 N7 O13
Mol. wt.	2583.89	1377.04
Crystal system	Monoclinic	Monoclinic
Space group	$P2_1/n$	$P2_1/c$
Temperature /K	150	296
Wavelength /Å	0.71073	0.71073
a /Å	10.3429(16)	10.2598(8)
b /Å	28.417(4)	17.9419(15)
c /Å	39.423(6)	34.346(3)
α/°	90	90
β/°	93.408(6)	94.262(3)
γ/°	90	90
V/ Å^3	11566(3)	6304.9(9)
Z	4	4
Density/Mgm^{-3}	1.484	1.451

Abs. Coeff. /mm^{-1}	0.803	0.743
F(000)	5276	2816
Refl. collected	255227	104782
Refl. unique	23693	13425
Max. 2θ/°	26.471	26.833
Ranges (h, k, l)	-12<= h <=12 -35 <= k <=33 -49<= l <=49	-13<= h <=13 -22<= k <=22 -43<= l <=43
Complete to 2θ (%)	99.3	99.3
Refl. with I > 2σ(I)	20709	8473
Data/Restraints/Parameters	23693/503/1492	13425/6/ 797
Goof (F^2)	1.087	1.053
R1 [I > 2s(I)]	0.0646	0.0532
wR2 [I > 2s(I)]	0.1492	0.1150
R1 [all data]	0.0746	0.1097
wR2 [all data]	0.1555	0.1370

Table S2: Selected bond distances (Å) and angles (°) for compounds 1-2	
1	Cd1-O10 2.165(4); Cd1-O2 2.201(4); Cd1-O6 2.213(4); Cd1-O4 2.276(4); Cd1-O3 2.429(4); Cd2-O1 2.247(4); Cd2-O5 2.277(5); Cd2-O9 2.211(4); Cd2-O17 2.302(6); Cd2-O18 2.285(5); Cd2-O19 2.269(7); Cd3-O12 2.207(4); Cd3-O14 2.216(4); Cd3-O8 2.283(4); Cd3-O16 2.303(3); Cd3-O15 2.371(4); Cd3-O7 2.503(4); Cd4-O7 2.329(4); Cd4-O11 2.208(4); Cd4-O13 2.208(5); Cd4-O20 2.298(7); Cd4-O21 2.275(7); Cd4-O22 2.286(7). <O10-Cd1-O2 102.68(18); <O10-Cd1-O6 136.86(17); <O2-Cd1-O6 98.76(18); <O10-Cd1-O4 110.92(16); <O2-Cd1-O4 93.27(14); <O6-Cd1-O4 104.65(17); <O10-Cd1-O3 92.98(17); <O2-Cd1-O3 148.63(15); <O6-Cd1-O3 87.45(18); <O4-Cd1-O3 55.54(13); <O9-Cd2-O1 97.80(19; <O9-Cd2-O19 88.4(3); <O1-Cd2-O19 89.7(3); <O9-Cd2-O5 94.10(17); <O1-Cd2-O5 94.60(18); <O19-Cd2-O5 174.7(3) ; <O9-Cd2-O18 93.48(19); <O1-Cd2-O18 168.2(2); <O19-Cd2-O18 87.0(3); <O5-Cd2-O18 88.2(2); <O9-Cd2-O17 174.8(3); <O1-Cd2-O17 83.4(2); <O19-Cd2-O17 86.5(4); <O5-Cd2-O17 90.9(3); <O18-Cd2-O17 85.0(2); <O12-Cd3-O14 97.89(16); <O12-Cd3-O8 147.19(14); <O14-Cd3-O8 91.32(14); <O12-Cd3-O16 100.21(15); <O14-Cd3-O16 92.85(13); <O8-Cd3-O16 110.75(14); <O12-Cd3-O15 96.62(16); <O14-Cd3-O15 147.78(14); <O8-Cd3-O15 91.86(14); <O16-Cd3-O15 56.23(12); <O12-Cd3-O7 92.57(14); <O14-Cd3-O7 109.56(14); <O8-Cd3-O7 54.78(13); <O16-Cd3-O7 152.45(13); <O15-Cd3-O7 98.33(13); <O11-Cd4-O13 109.1(2); <O11-Cd4-O21 87.4(3); <O13-Cd4-O21 163.3(3); <O11-Cd4-O22 167.7(3); <O13-Cd4-O22 81.6(3); <O21-Cd4-O22 81.7(4); <O11-Cd4-O20 87.1(2); <O13-Cd4-O20 84.8(3); <O21-Cd4-O20 93.6(4); <O22-Cd4-O20 88.0(3); <O11-Cd4-O7 91.12(15); <O13-Cd4-O7 84.81(17); <O21-Cd4-O7 97.9(3); <O22-Cd4-O7 95.9(3); <O20-Cd4-O7 168.3(3).
2	Cd1-O5 2.200(3); Cd1-O2 2.255(4); Cd1-O4 2.254(3); Cd1-O7 2.313(3); Cd1-O8 2.470(3); Cd1-O1 2.481(4); Cd2-O6 2.222(4); Cd2-O3 2.230(4); Cd2-O9 2.272(4); Cd2 -O10 2.275(4); Cd2-O8 2.277(3); Cd2-O11 2.298(4).

	<O5-Cd1-O2 101.58(15); <O5-Cd1-O4 91.57(15); <O2-Cd1-O4 89.30(13); <O5-Cd1-O7 147.41(13); <O2-Cd1-O7 103.95(14); <O4-Cd1-O7 108.57(15); <O5-Cd1-O8 93.48(12); <O2-Cd1-O8 148.21(13); <O4-Cd1-O8 118.37(12); <O7-Cd1-O8 54.60(12); <O5-Cd1-O1 90.38(15); <O2-Cd1-O1 54.58(13); <O4-Cd1-O1 143.39(13); <O7-Cd1-O1 88.17(15); <O8-Cd1-O1 97.98(12); <O6-Cd2-O3 102.07(16); <O6-Cd2-O9 172.20(16); <O3-Cd2-O9 85.02(17); <O6-Cd2-O10 87.60(16); <O3-Cd2-O10 168.21(16); <O9-Cd2-O10 84.99(18); <O6-Cd2-O8 88.01(14); <O3-Cd2-O8 85.40(14); <O9-Cd2-O8 95.87(15); <O10-Cd2-O8 101.85(15); <O6-Cd2-O11 87.03(18); <O3-Cd2-O11 88.30(17); <O9-Cd2-O11 89.97(18); <O10-Cd2-O11 85.45(18); <O8-Cd2-O11 171.00(16).

Table S3: Hydrogen bond geometry (Å, °) in compounds 1-2

Compound	D-H···A	D···H (Å)	H···A (Å)	D···A (Å)	<D−H···A(°)
1	N1-H1N···O25	0.88	1.97	2.848(8)	172
	N3-H3N···O24	0.88	2.18	2.976(8)	150
	C54-H54···O24	0.95	2.51	3.299(8)	141
	C106-H10F···N11	0.98	2.68	3.650(2)	171
	C106-H10H···O15	0.98	2.60	3.349(13)	134
	C105-H105···O20	0.95	2.60	3.330(2)	134
	C104-H10M···O23	0.98	2.46	3.340(3)	150
	C103-H10P···O15	0.98	2.41	3.327(15)	156
	C113-H11F···O5	0.98	2.26	3.220(2)	169
	C126-H12E···N11A	0.98	1.59	2.310(6)	126
	C126-H12F···N10	0.98	2.91	3.730(8)	142
2	N1-H1N···O13	0.80	2.20	2.921(8)	161
	N2-H2N···O12	0.86	2.53	3.327(8)	154
	C33-H33···O12	0.93	2.56	3.400(7)	151
	C54-H54···O6	0.93	2.37	3.054(8)	130
	C61-H61A···O4	0.96	2.42	3.356(9)	165
	C51-H51···O11	0.93	2.58	3.181(10)	123
	C64-H64A···O4	0.96	2.54	3.303(10)	137
	C64-H64B···O2	0.96	2.52	3.371(10)	148