Supporting Information

Samarium Doped Cobalt Metal-Organic Framework as a Versatile Catalyst for the Conversion of Furfural and 2-Methyl Furan to High-Value Added Biofuel Precursor

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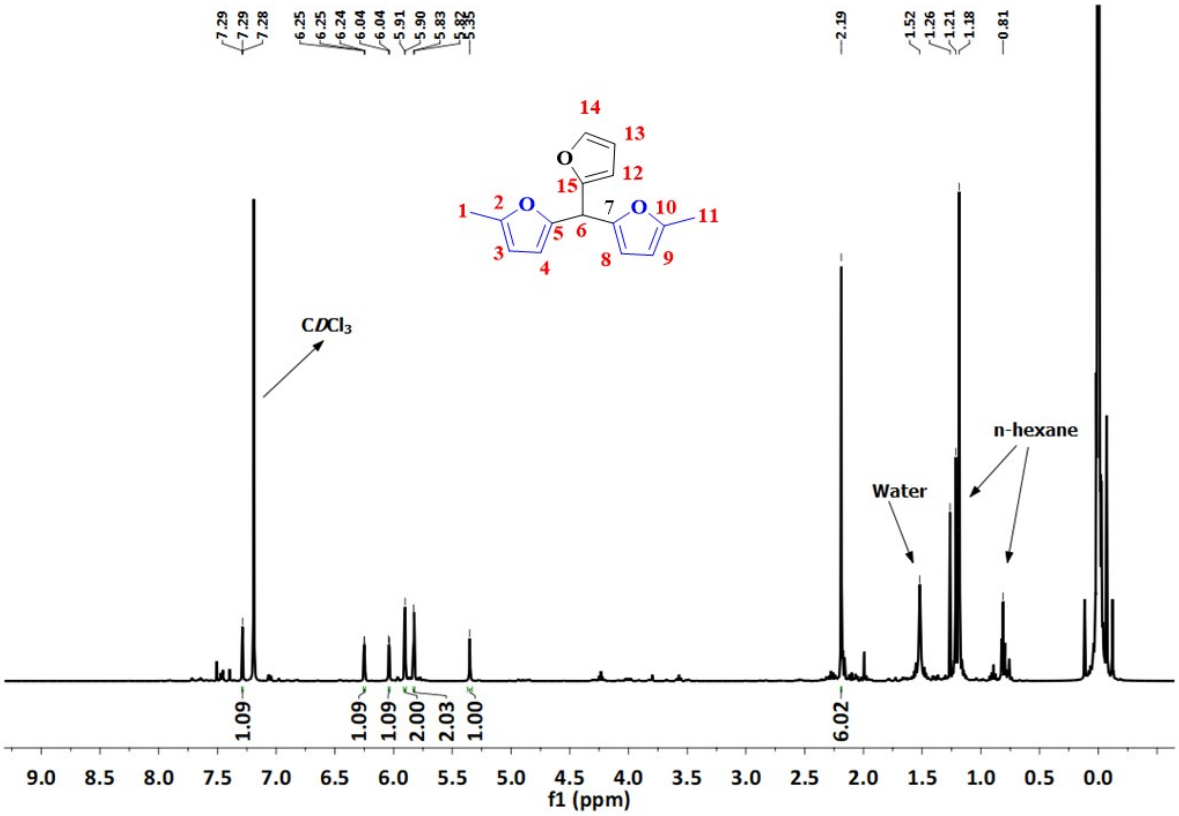
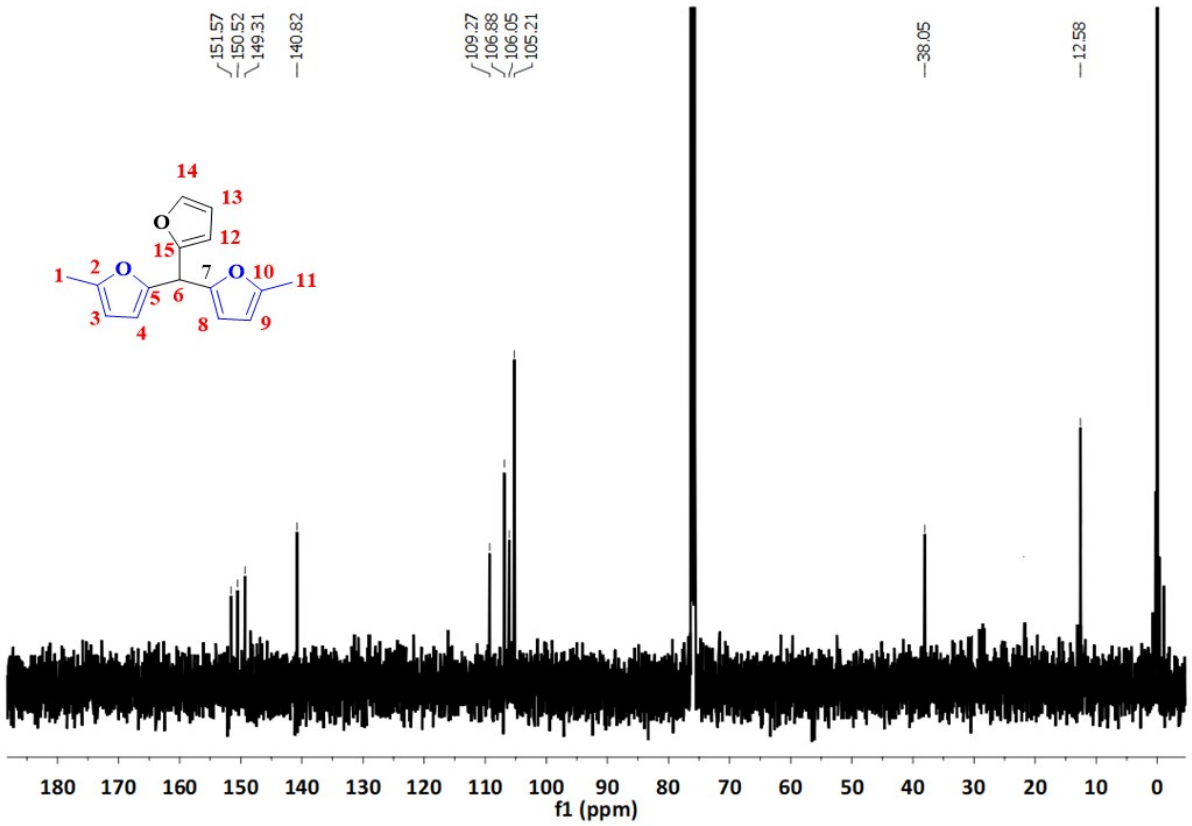


^{1}H NMR ($CDCl_3$, 500 MHz): 2.19 (s, 6H, H^{1} H^{11}), 5.35 (s,1H, H^{6}), 5.82 (d, 2H, H^{4} H^{8}), 5.91 (d, 2H, H^{3} H^{9}), 6.04 (d, 2H, H^{12}), 6.24-6.25 (m, 1H, H^{13}), 7.28 (d, 1H, H^{14})

Figure S1. ^{1}H NMR Spectrum of 5,5′-(furan-2-ylmethylene)bis(2-methylfuran).



^{13}C NMR ($CDCL_3$, 125 MHz): 12.58 (C^1, C^{11}), 38.05(C^6), 105.21(C^3, C9), 106.059(C^{12}), 107.88(C^4, C^8), 109.27(C^{13}), 140.82 (C^{14}), 149.31(C^2, C^{10}), 150.52(C^5, C^7), 151.57(C^{15})

Figure S2. ^{13}C NMR Spectrum of 5,5′-(furan-2-ylmethylene)bis(2-methylfuran).

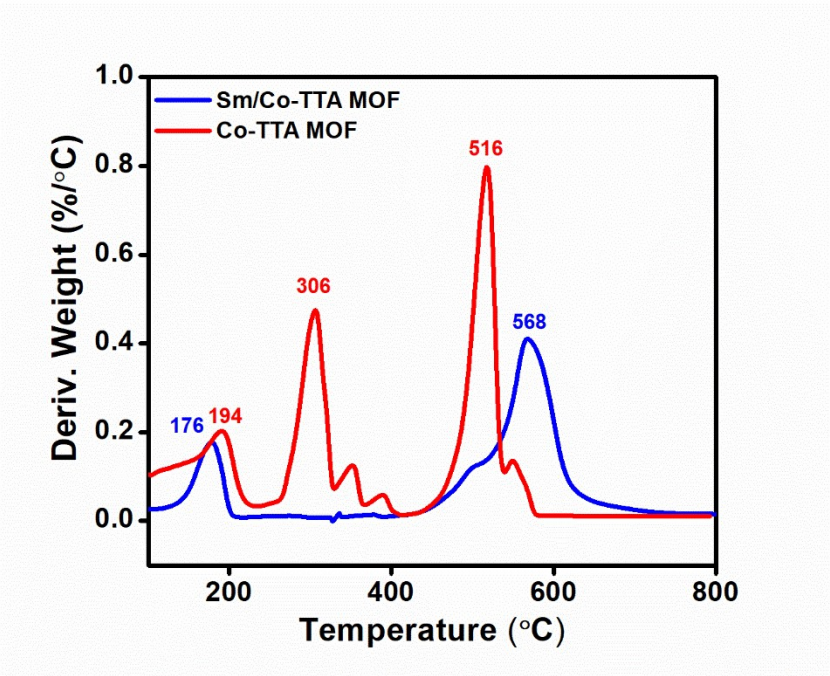


Figure S3. DTG Curve of Co-TTA MOF and Sm/Co-TTA MOF.

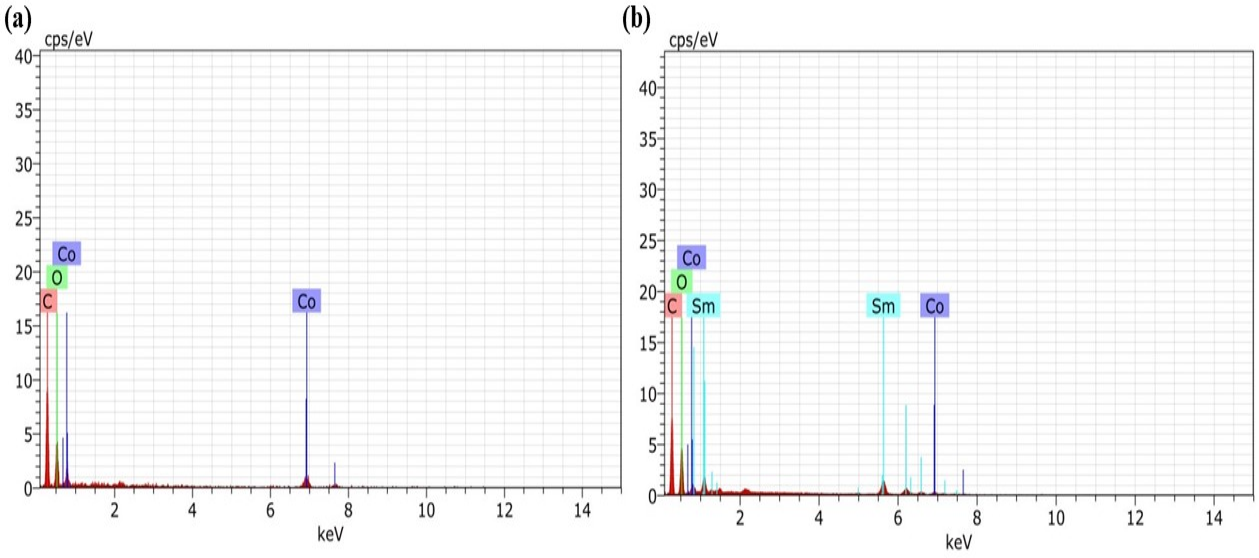


Figure S4. EDAX of Co-TTA and Sm/Co-TTA MOF.

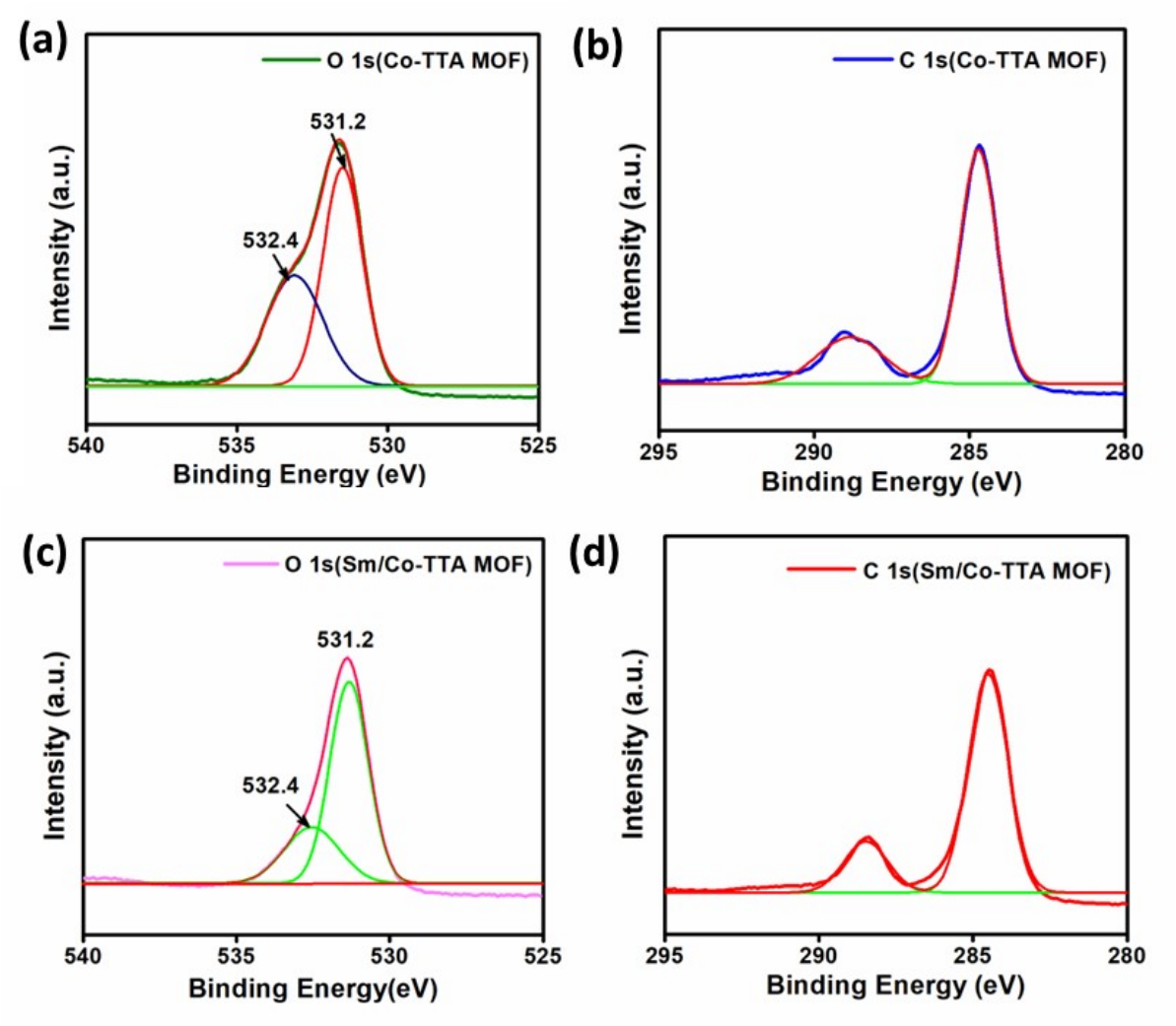


Figure S5. XPS of **(a)** O 1s of Co-TTA MOF , **(b)** C 1s of Co-TTA MOF , **(c)** O 1s of SM/Co-TTA MOF, **(d)** C 1s of Sm/Co-TTA MOF.

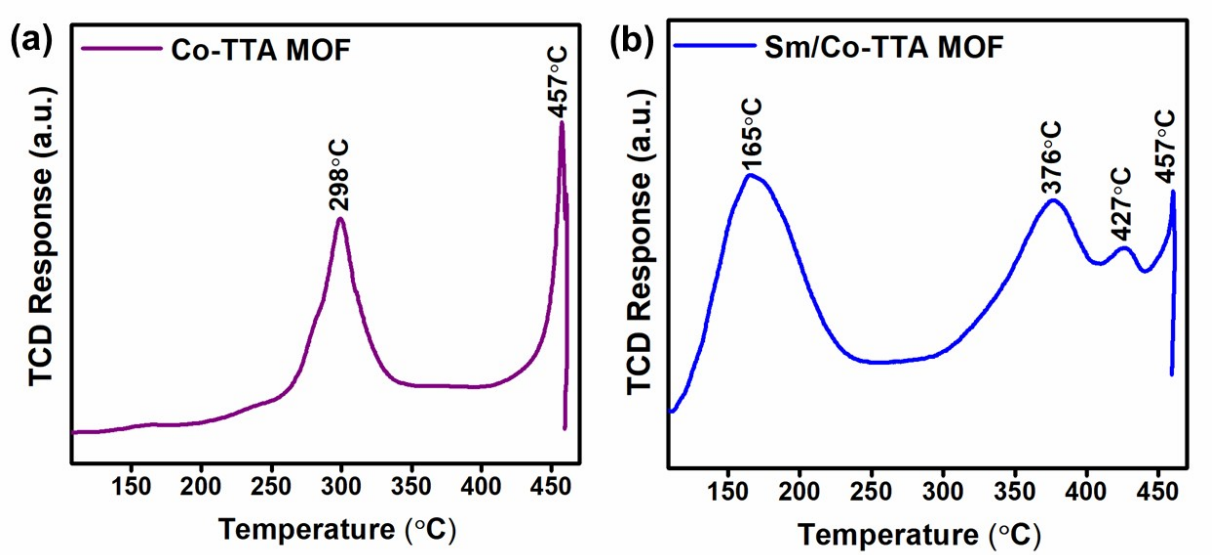


Figure S6. NH_3-TPD Profiles of (a) Co-TTA MOF , (b) Sm/Co-TTA MOF.

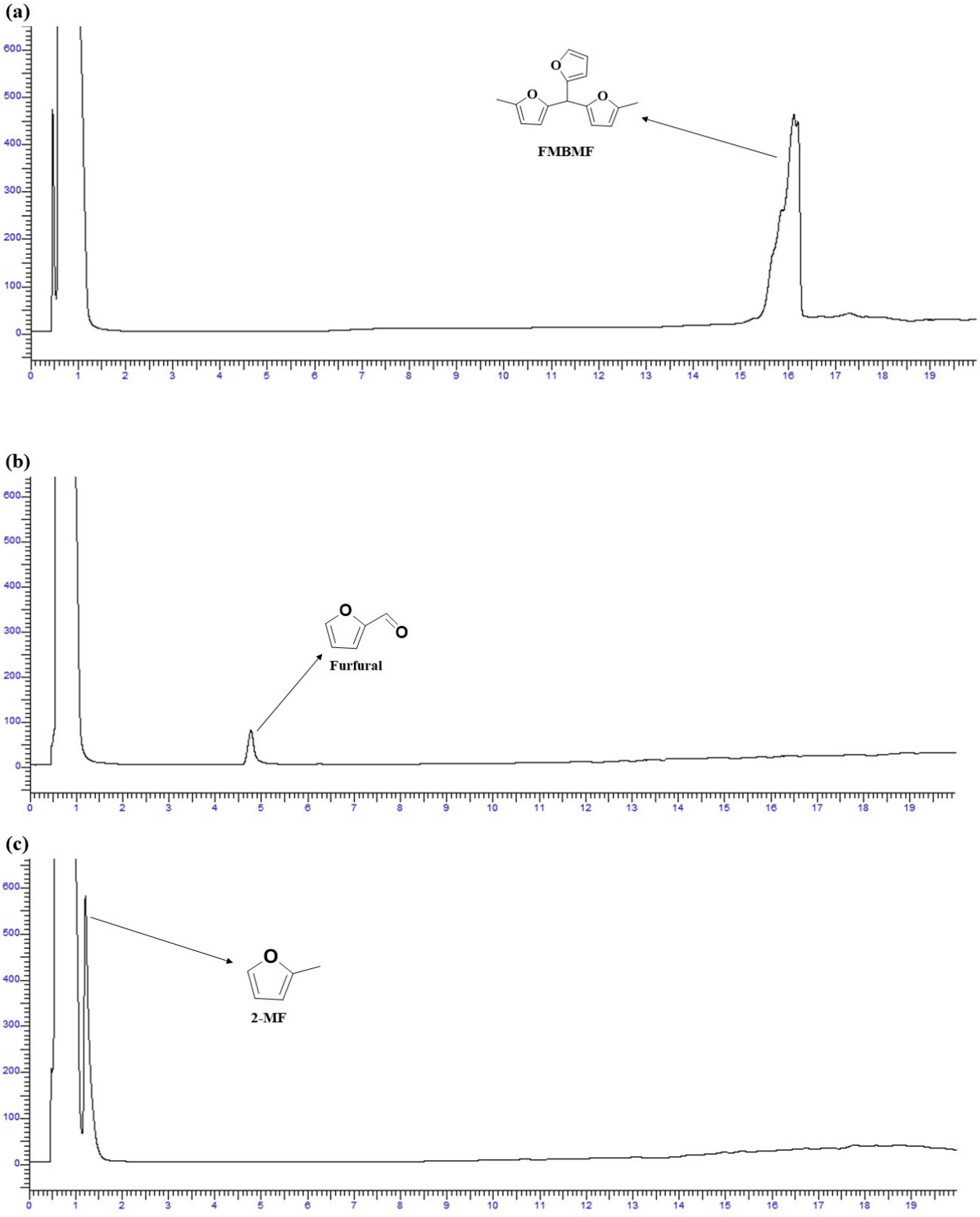


Figure S7. GC Chromatogram of (a) FMBMF , (b) Furfural , (c) 2 MF

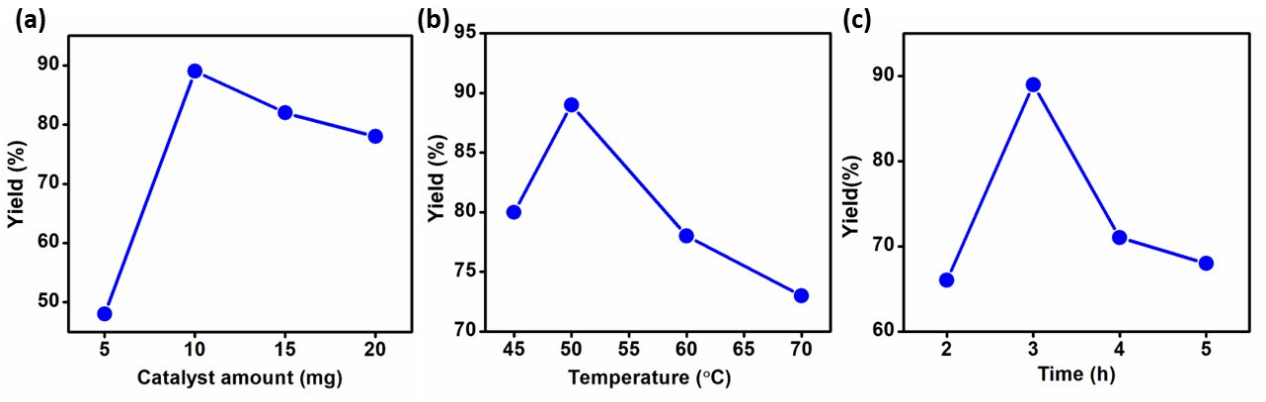


Figure S8. (a) Kinetic curve of formation of FMBMF by different amounts of catalyst. **(b)** The kinetic curve of FMBMF formation at different temperature rates. **(c)** The kinetic curve of FMBMF formation at different time intervals.

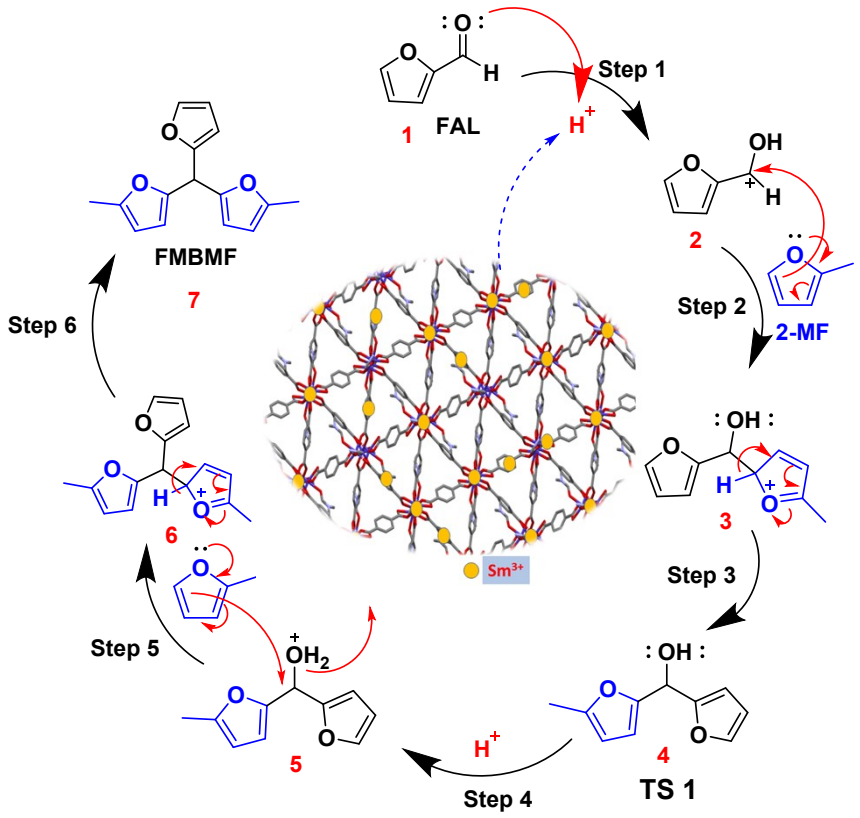


Figure S9. Proposed mechanism of catalytic conversion of FAL and 2-MF to FMBMF.

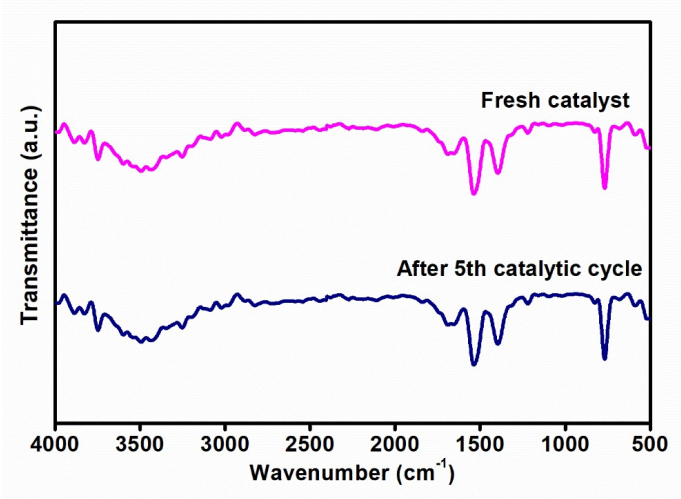


Figure S10. FTIR Spectra of Fresh Sm/Co-TTA MOF and after 5 th catalytic cycle.

Table S1. Crystal data and structure refinement for Co-TTA MOF.

Parameter	**Co-TTA MOF**	**Parameter**	**Co-TTA MOF**
Empirical formula	$C_{18}H_{19}Co_{1.5}N_2O_8$	μ/mm^{-1}	1.237
Formula weight	479.75	F(000)	982.0
Temperature/K	293(2)	Crystal size/mm^3	0.3 × 0.1 × 0.1
Crystal system	monoclinic	Radiation	MoKα (λ = 0.71073)
Space group	$P2_1/n$	2Θ range for data collection/°	5.388 to 56.064
a/Å	14.7519(12)	Index ranges	-18 ≤ h ≤ 19, -11 ≤ k ≤ 12, -19 ≤ l ≤ 19
b/Å	9.6628(7)	Reflections collected	13904
c/Å	15.4954(12)	Independent reflections	4752 [R_{int} = 0.0810, R_{sigma} = 0.0873]
α/°	90	Data/restraints/parameters	4752/76/271
β/°	106.904(3)	Goodness-of-fit on F^2	1.193
γ/°	90	Final R indexes [I>=2σ (I)]	R1 = 0.1065, wR2 = 0.3073
Volume/Å^3	2113.4(3)	Final R indexes [all data]	R1 = 0.1510, wR2 = 0.3572
Z	4	Largest diff. peak/hole / e Å-3	2.04/-1.64
ρ_{calc}g/cm^3	1.508		

Table S2. Selected Bond length(A°) and Bond angle for Co-TTA MOF.

Bond	Length(A°)	Bond	Length(A°)
Co2- O2	2.039(5)	Co1- O1	1.995(6)
Co2- O2[1]	2.039(5)	Co1- O7[2]	2.005(6)
Co2- O3	2.143(5)	Co1- O4	2.264(6)
Co2- O3[1]	2.143(5)	Co1- O5	2.226(10)
Co2- O8[2]	2.057(5)	Co1- O6	2.007(9)
Co1- O3	2.106(5)	Co2- O8[3]	2.057(5)

Bond	Angle/°	Bond	Angle/°	Bond	Angle/°
O2-Co2-O2[1]	180.0	O8[2]-Co2-O3[1]	88.9(2)	O1-Co1-O5	84.1(4)
O2-Co2-O3	88.25(19)	O8[3]-Co2-O3[1]	91.1(2)	O1-Co1-O6	103.9(4)
O2-Co2-O3[1]	91.75(19)	O8[2]-Co2-O3	91.1(2)	O7[2]-Co1-O3	102.6(2)
O2[1]-Co2-O3	91.75(19)	O8[3]-Co2-O3	88.9(2)	O7[2]-Co1-O4	94.7(3)
O2[1]-Co2-O3[1]	88.25(19)	O8[2]-Co2-O8[3]	180.0	O7[2]-Co1-O5	170.5(4)
O2-Co2-O8[2]	93.9(2)	O3-Co1-O4	59.6(2)	O7[2]-Co1-O6	89.4(4)
O2[1]-Co2-O8[3]	93.9(2)	O3-Co1-O5	83.8(3)	C1-O2-Co2	140.5(5)
O2[1]-Co2-O8[2]	86.1(2)	O1-Co1-O3	96.6(2)	Co1-O3-Co2	108.5(2)
O2-Co2-O8[3]	86.1(2)	O1-Co1-O7[2]	102.0(3)	C2-O3-Co2	128.7(5)
O3-Co2-O3[1]	180.0(2)	O6-Co1-O5	81.9(5)	C2-O3-Co1	94.1(5)
O1-Co1-O4	153.7(3)	O5-Co1-O4	82.4(4)	C2-O3-Co1	94.1(5)

Table S3. Optimization Reactions for Co-TTA MOF.

S.No.	Catalyst Amount(mg)	Temperature (^{o}C)	Time(h)	Yield (%)
1.	10	50	3	43
2.	15	50	3	39
3.	10	40	3	31
4.	10	60	3	44
5.	10	50	4	41
6.	10	50	5	36