Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information

Construction of a series of pH stable Ca-based MOFs, their CO_2 adsorption and catalytic activity

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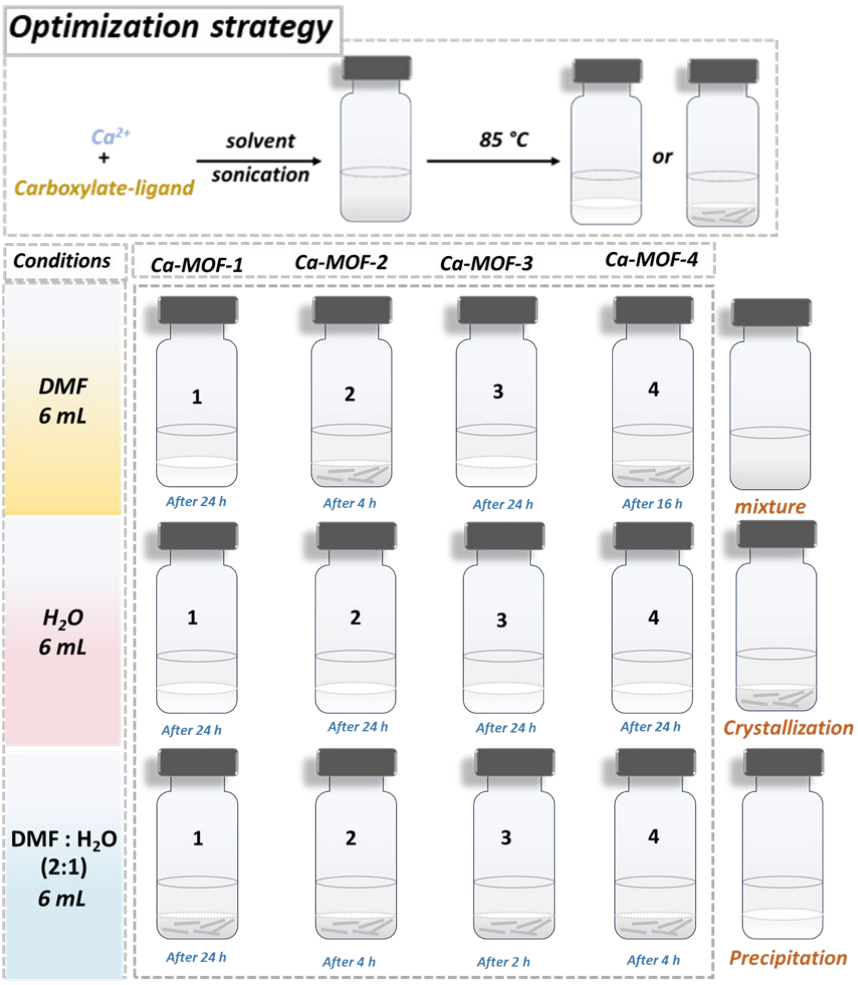


Scheme S1. Optimization synthesis strategy for the crystallization of four Ca-based MOFs. Reaction conditions: metal: ligand = 2:1, solvent 6 ml (DMF: H_2O = 2:1).

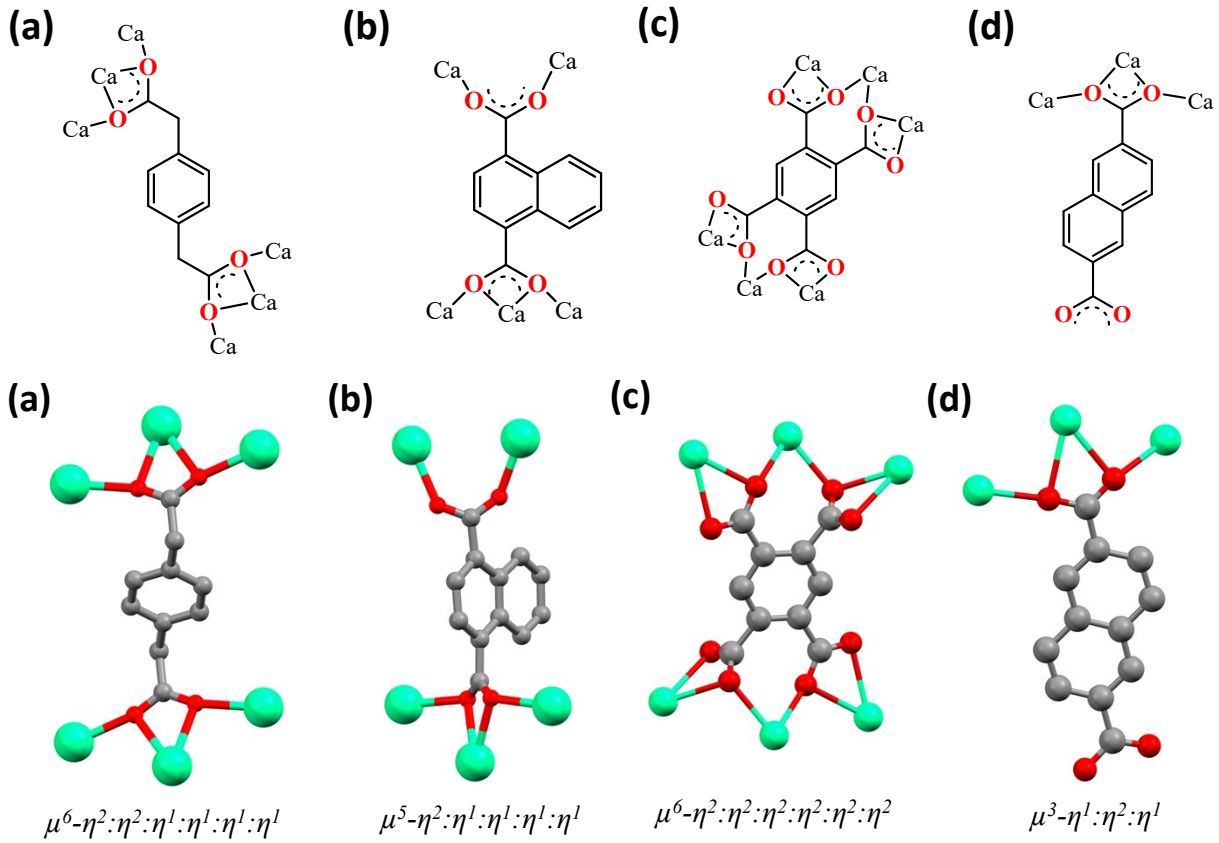


Figure S1. Different bridging coordination modes of the carboxylate groups of each ligand in **Ca-MOF 1-4**.

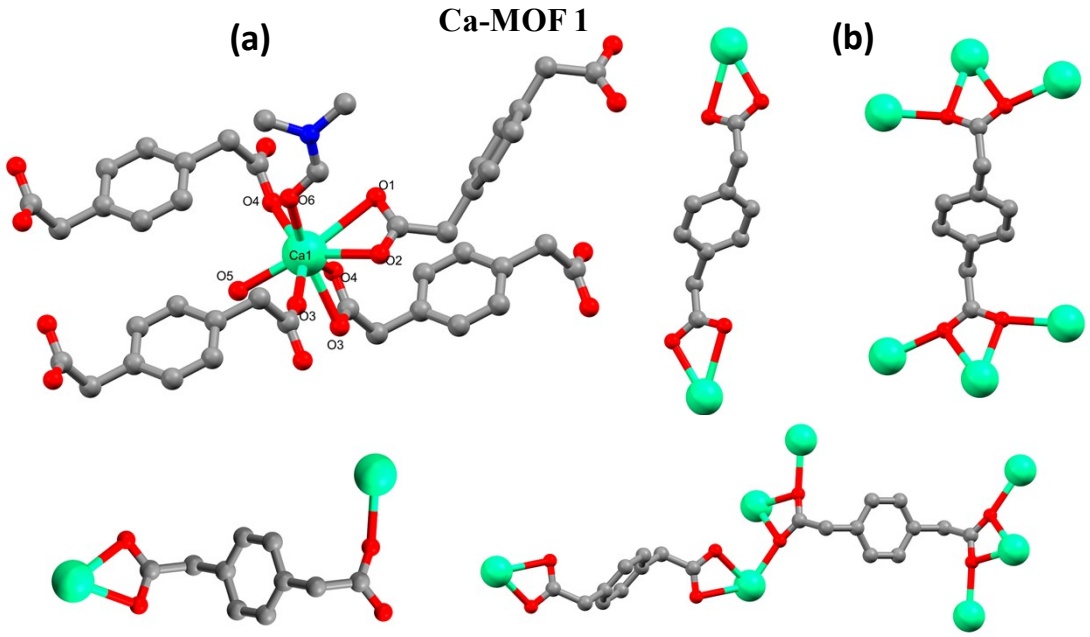


Figure S2. (a) Coordination environment of Ca(II), (b) different coordination mode of the carboxylate groups of PDA ligand in **Ca-MOF 1**.

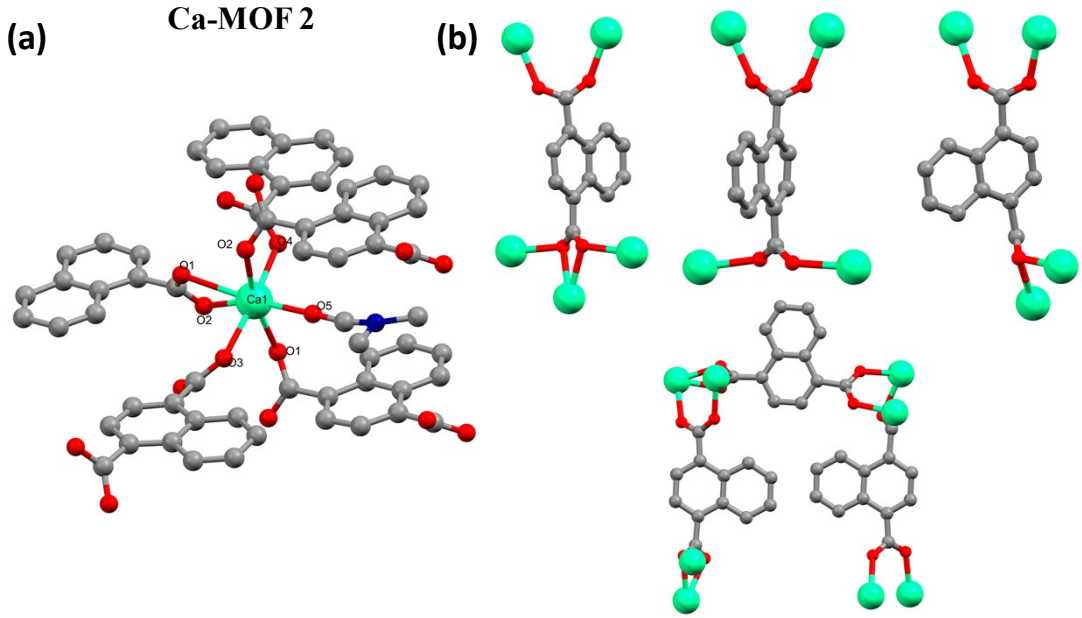
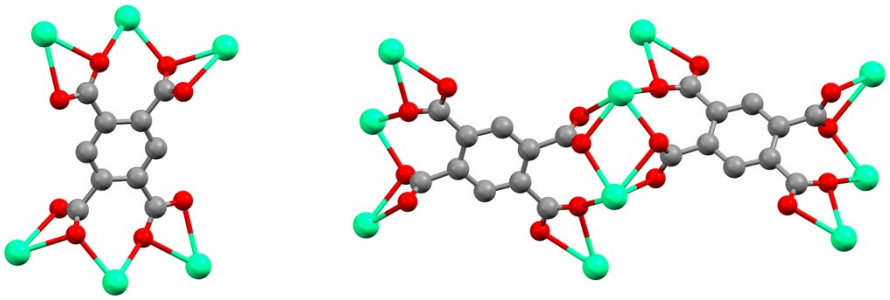


Figure S3. (a) Coordination environment of Ca(II), (b) different coordination mode of the carboxylate groups of 1,4 NDC ligand in **Ca-MOF 2**.

Ca-MOF 3



Ca-MOF 4

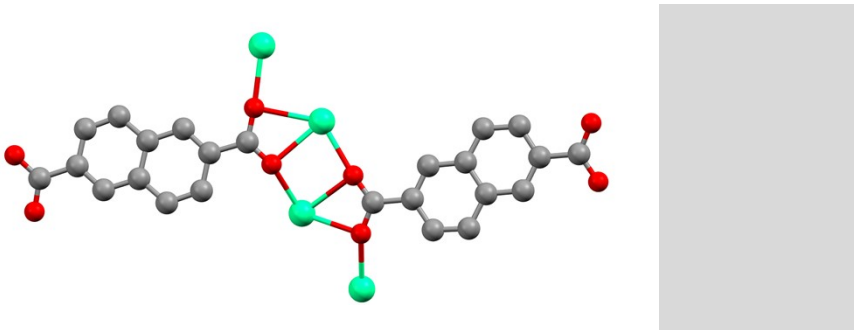


Figure S4. Different coordination modes of the carboxylate groups of each ligand in **Ca-MOF 3-4**.

Table S1. Crystal and Structure Refinement Data for **Ca-MOF (1-4)**.

CCDC No.	2234284	2234285	2284521	2284522
empirical formula	$C_{13}H_{17}CaNO_6$	$C_{15.01}H_{13.13}CaN_{0.98}O_5$	$C_{13.05}H_{15.05}Ca_2NO_{12}$	$C_{24}H_{24}Ca_2O_{14}$
formula weight	323.35	327.32	458.07	616.59
temperature/K	145.0	144.95	166.52	145.26
crystal system	triclinic	orthorhombic	triclinic	triclinic
space group	P-1	$P2_12_12_1$	P-1	P1
a/Å	6.7506(13)	6.6525(13)	9.2135(19)	6.527(18)
b/Å	10.564(2)	14.409(3)	10.112(2)	7.215(18)
c/Å	10.746(2)	14.878(4)	10.455(2)	13.83(5)
α/°	77.010(7)	90	96.156(8)	74.90(13)
β/°	82.594(6)	90	98.994(7)	76.50(8)

γ/°	81.892(6)	90	113.548(7)	89.9(2)
volume/Å^3	735.5(2)	1426.2(5)	866.3(3)	610(3)
Z	2	4	2	1
ρ_{calc}(g/cm^3)	1.460	1.524	1.756	1.678
μ/mm^{-1}	0.453	0.463	0.727	0.545
F(000)	340.0	680.0	473.0	320.0
crystal size/mm^3	0.4 × 0.3 × 0.2	0.4 × 0.3 × 0.2	0.4 × 0.3 × 0.2	0.4 × 0.3 × 0.2
radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
2θ range for data collection/°	4.96 to 49.996	5.654 to 50	4.474 to 49.998	5.86 to 68.93
index ranges	-8 ≤ h ≤ 8, -12 ≤ k ≤ 12, -12 ≤ l ≤ 12	-7 ≤ h ≤ 7, -14 ≤ k ≤ 17, -17 ≤ l ≤ 17	-9 ≤ h ≤ 10, -12 ≤ k ≤ 12, -12 ≤ l ≤ 12	-9 ≤ h ≤ 10, -10 ≤ k ≤ 11, -21 ≤ l ≤ 21
reflections collected	5555	13214	7790	8117
independent reflections	2550 [R_{int} = 0.0456, R_{sigma} = 0.0665]	2492 [R_{int} = 0.0660, R_{sigma} = 0.0444]	2971 [R_{int} = 0.0525, R_{sigma} = 0.0593]	6080 [R_{int} = 0.0800, R_{sigma} = 0.2056]
data/restraints/ parameters	2550/0/193	2492/0/235	2971/1/272	6080/5/310
goodness-of-fit on F^2	1.063	1.044	1.033	1.056
final R indexes [I ≥ 2σ (I)]	R_1 = 0.0538, wR_2 = 0.1273	R_1 = 0.0313, wR_2 = 0.0687	R_1 = 0.0398, wR_2 = 0.1055	R_1 = 0.0868, wR_2 = 0.1585
final R indexes [all data]	R_1 = 0.0755, wR_2 = 0.1385	R_1 = 0.0395, wR_2 = 0.0735	R_1 = 0.0423, wR_2 = 0.1076	R_1 = 0.1659, wR_2 = 0.1986
largest diff. peak/hole/e.Å^{-3}	0.76/-0.34	0.20/-0.31	0.58/-1.41	0.92/-1.43

Table S2. Bond Lengths (Å) for **Ca-MOF 1**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Ca1	$Ca1^{1}$	3.9003(14)	Ca1	O2	2.432(2)
Ca1	$Ca1^{2}$	3.9651(13)	Ca1	O1	2.800(3)
Ca1	$O4^{2}$	2.492(2)	Ca1	O5	2.378(2)
Ca1	$O4^{3}$	2.370(2)	Ca1	O6	2.407(2)
Ca1	O3	2.364(2)	Ca1	$C10^{2}$	2.906(3)
Ca1	$O3^{2}$	2.594(2)			

Symmetry transformations used to generate equivalent atoms: ^{1}2-X,1-Y,1-Z; ^{2}1-X,1-Y,1-Z; ^{3}1+X,+Y,+Z.

Table S3. Bond Angles (°) for **Ca-MOF 1**.

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
$Ca1^{1}$	Ca1	$Ca1^{2}$	118.24(3)	$Ca1^{1}$	Ca1	$Ca1^{2}$	118.24(3)
$O4^{3}$	Ca1	$Ca1^{1}$	37.74(5)	$O4^{3}$	Ca1	$Ca1^{1}$	37.74(5)
$O4^{2}$	Ca1	$Ca1^{1}$	35.60(5)	$O4^{2}$	Ca1	$Ca1^{1}$	35.60(5)
$O4^{2}$	Ca1	$Ca1^{2}$	86.05(5)	$O4^{2}$	Ca1	$Ca1^{2}$	86.05(5)
$O4^{3}$	Ca1	$Ca1^{2}$	148.35(6)	$O4^{3}$	Ca1	$Ca1^{2}$	148.35(6)
$O4^{3}$	Ca1	$O4^{2}$	73.34(8)	$O4^{3}$	Ca1	$O4^{2}$	73.34(8)
$O4^{2}$	Ca1	$O3^{2}$	51.27(7)	$O4^{2}$	Ca1	$O3^{2}$	51.27(7)
$O4^{3}$	Ca1	$O3^{2}$	121.38(7)	$O4^{3}$	Ca1	$O3^{2}$	121.38(7)
$O4^{3}$	Ca1	O2	128.29(8)	$O4^{3}$	Ca1	O2	128.29(8)
$O4^{3}$	Ca1	O1	79.27(7)	$O4^{3}$	Ca1	O1	79.27(7)
$O4^{2}$	Ca1	O1	72.84(7)	$O4^{2}$	Ca1	O1	72.84(7)
$O4^{3}$	Ca1	O5	78.83(8)	$O4^{3}$	Ca1	O5	78.83(8)
$O4^{3}$	Ca1	O6	84.14(8)	$O4^{3}$	Ca1	O6	84.14(8)
$O4^{3}$	Ca1	$C10^{2}$	98.17(8)	$O4^{3}$	Ca1	$C10^{2}$	98.17(8)
$O4^{2}$	Ca1	$C10^{2}$	25.74(7)	$O4^{2}$	Ca1	$C10^{2}$	25.74(7)
$O3^{2}$	Ca1	$Ca1^{2}$	34.95(5)	$O3^{2}$	Ca1	$Ca1^{2}$	34.95(5)
$O3^{2}$	Ca1	$Ca1^{1}$	85.22(5)	$O3^{2}$	Ca1	$Ca1^{1}$	85.22(5)
O3	Ca1	$Ca1^{2}$	38.94(5)	O3	Ca1	$Ca1^{2}$	38.94(5)
O3	Ca1	$Ca1^{1}$	152.25(6)	O3	Ca1	$Ca1^{1}$	152.25(6)
O3	Ca1	$O4^{3}$	148.90(9)	O3	Ca1	O1	127.93(8)
O3	Ca1	$O4^{2}$	124.81(7)	O3	Ca1	O5	76.83(8)
O3	Ca1	$O3^{2}$	73.89(8)	O3	Ca1	O6	85.93(8)

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
O3	Ca1	O2	80.25(8)	O3[2]	Ca1	C10[2]	25.67(7)
O3[2]	Ca1	O1	98.74(7)	O3	Ca1	C10[2]	99.56(8)
O2	Ca1	Ca1[1]	111.90(6)	O2	Ca1	Ca1[2]	73.90(6)
O2	Ca1	O4[2]	89.68(8)	O1	Ca1	Ca1[1]	72.45(5)
O2	Ca1	O3[2]	74.35(8)	O1	Ca1	Ca1[2]	117.77(6)
O2	Ca1	O1	49.02(7)	O1	Ca1	C10[2]	83.73(8)
O2	Ca1	C10[2]	79.27(8)	O5	Ca1	Ca1[2]	76.94(6)
O5	Ca1	Ca1[1]	82.45(6)	O5	Ca1	O2	150.83(8)
O5	Ca1	O4[2]	88.77(8)	O5	Ca1	O1	154.68(8)
O5	Ca1	O3[2]	82.08(8)	O5	Ca1	O6	109.33(8)

Symmetry transformations used to generate equivalent atoms: [1]2-X,1-Y,1-Z; [2]1-X,1-Y,1-Z; [3]1+X,+Y,+Z.

Table S4. Bond Lengths (Å) for **Ca-MOF 2**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Ca1	Ca1[1]	3.8839(9)	Ca1	O4	2.332(2)
Ca1	Ca1[2]	3.8839(9)	Ca1	O3[2]	2.315(2)
Ca1	O2[3]	2.487(2)	Ca1	O5	2.280(3)
Ca1	O2[4]	2.435(2)	Ca1	C1[3]	2.867(3)
Ca1	O1[5]	2.456(2)	Ca1	O1[3]	2.544(2)

Symmetry transformations used to generate equivalent atoms: [1]1/2+X,3/2-Y,1-Z; [2]-1/2+X,3/2-Y,1-Z; [3]1-X,1/2+Y,1/2-Z; [4]3/2-X,1-Y,1/2+Z; [5]1/2-X,1-Y,1/2+Z.

Table S5. Bond Angles (°) for **Ca-MOF 2**.

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
Ca1[1]	Ca1	Ca1[2]	117.83(3)	O1[5]	Ca1	O1[3]	121.41(7)
O2[3]	Ca1	Ca1[2]	37.43(5)	O1[3]	Ca1	C1[3]	26.16(8)
O2[4]	Ca1	Ca1[1]	38.37(5)	O1[5]	Ca1	C1[3]	96.57(9)
O2[4]	Ca1	Ca1[2]	152.11(6)	O4	Ca1	Ca1[1]	70.26(7)
Ca1[6]	O2	Ca1[7]	104.20(8)	O4	Ca1	Ca1[2]	107.14(7)
C1	O2	Ca1[6]	134.7(2)	O4	Ca1	O2[4]	80.56(9)
C1	O2	Ca1[7]	94.05(19)	O4	Ca1	O2[3]	85.23(9)
Ca1[8]	O1	Ca1[7]	101.90(8)	O4	Ca1	O1[5]	97.55(9)
O2[3]	Ca1	Ca1[1]	82.18(6)	O4	Ca1	O1[3]	92.52(8)
O2[4]	Ca1	O2[3]	120.19(7)	O4	Ca1	C1[3]	88.03(9)

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
O2[4]	Ca1	O1[3]	70.71(7)	O3[2]	Ca1	Ca1[2]	65.06(6)
O2[3]	Ca1	O1[3]	52.19(7)	O3[2]	Ca1	Ca1[1]	109.25(7)
O2[4]	Ca1	O1[5]	167.87(8)	O3[2]	Ca1	O2[3]	86.09(8)
O2[4]	Ca1	C1[3]	95.34(9)	O3[2]	Ca1	O2[4]	104.55(9)
O2[3]	Ca1	C1[3]	26.04(9)	O3[2]	Ca1	O1[3]	82.73(9)
O1[3]	Ca1	Ca1[2]	82.04(6)	O3[2]	Ca1	O1[5]	78.91(8)
O1[5]	Ca1	Ca1[2]	39.87(5)	O3[2]	Ca1	O4	171.29(9)
O1[5]	Ca1	Ca1[1]	151.85(6)	O3[2]	Ca1	C1[3]	84.50(9)
O1[3]	Ca1	Ca1[1]	38.23(5)	O5	Ca1	Ca1[2]	121.36(8)
O1[5]	Ca1	O2[3]	71.34(7)	O5	Ca1	Ca1[1]	120.59(8)
C1	O1	Ca1[8]	131.8(2)	O5	Ca1	O2[3]	156.46(10)
C1	O1	Ca1[7]	91.32(18)	O5	Ca1	O2[4]	83.14(9)
C12	O4	Ca1	129.8(2)	O5	Ca1	O1[3]	150.49(10)
C12	O3	Ca1[1]	138.2(2)	O5	Ca1	O1[5]	85.18(10)
C13A	O5	Ca1	141.1(6)	O5	Ca1	O4	96.52(10)
C13B	O5	Ca1	178.5(5)	O5	Ca1	O3[2]	91.14(11)
O2	C1	Ca1[7]	59.91(16)	O5	Ca1	C1[3]	174.88(11)
O1	C1	Ca1[7]	62.51(16)	C1[3]	Ca1	Ca1[2]	59.02(8)
C2	C1	Ca1[7]	175.4(2)	C1[3]	Ca1	Ca1[1]	58.82(8)
O5	Ca1	Ca1[1]	82.45(6)	O5	Ca1	O2	150.83(8)
O5	Ca1	O4[2]	88.77(8)	O5	Ca1	O1	154.68(8)
O5	Ca1	O3[2]	82.08(8)	O5	Ca1	O6	109.33(8)

Symmetry transformations used to generate equivalent atoms: [1]1/2+X,3/2-Y,1-Z; [2]-1/2+X,3/2-Y,1-Z; [3]1-X,1/2+Y,1/2-Z; [4]3/2-X,1-Y,1/2+Z; [5]1/2-X,1-Y,1/2+Z; [6]3/2-X,1-Y,-1/2+Z; [7]1-X,-1/2+Y,1/2-Z; [8]1/2-X,1-Y,-1/2+Z.

Table S6. Bond Lengths (Å) for **Ca-MOF 3**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Ca2	Ca2[1]	3.8924(13)	Ca2	O7[1]	2.473(2)
Ca2	Ca1	3.9490(11)	Ca2	O7	2.387(2)
Ca2	O8[1]	2.492(2)	Ca2	O3	2.602(2)
Ca2	O4	2.437(2)	Ca2	O9	2.399(2)

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Ca2	O6	2.381(2)	Ca2	O10	2.401(2)
Ca2	C10[1]	2.828(3)	Ca1	O1[3]	2.577(2)
Ca1	Ca1[2]	3.9323(13)	Ca1	O5	2.450(2)
Ca1	O4	2.381(2)	Ca1	O11	2.409(2)
Ca1	O2[3]	2.521(2)	Ca1	O12	2.314(2)
Ca1	O2[4]	2.434(2)	Ca1	C1[3]	2.894(3)
Ca1	O6	2.655(2)			

Symmetry transformations used to generate equivalent atoms: [1]2-X,1-Y,1-Z; [2]1-X,-Y,-Z; [3]+X,-1+Y,+Z; [4]1-X,1-Y,-Z; [5]2-X,-Y,1-Z.

Table S7. Bond Angles (°) for **Ca-MOF 3**.

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
Ca2[1]	Ca2	Ca1	130.68(2)	O1[3]	Ca1	O6	83.49(7)
O8[1]	Ca2	Ca2[1]	87.14(5)	O1[3]	Ca1	C1[3]	25.94(7)
O8[1]	Ca2	Ca1	116.24(5)	O5	Ca1	Ca2	68.19(6)
O8[1]	Ca2	O3	73.15(7)	O5	Ca1	Ca1[2]	78.51(5)
O8[1]	Ca2	C10[1]	26.49(7)	O5	Ca1	O2[3]	82.02(7)
O4	Ca2	Ca2[1]	128.56(5)	O5	Ca1	O6	51.35(7)
O4	Ca2	Ca1	34.49(5)	O5	Ca1	O1[3]	76.97(8)
O4	Ca2	O8[1]	82.11(7)	O5	Ca1	C1[3]	74.87(8)
O4	Ca2	O7[1]	122.36(7)	O11	Ca1	Ca2	78.10(8)
O4	Ca2	O3	51.95(7)	O11	Ca1	Ca1[2]	152.09(8)
O4	Ca2	C10[1]	101.10(7)	O11	Ca1	O2[3]	120.33(9)
O6	Ca2	Ca2[1]	115.14(5)	O11	Ca1	O2[4]	154.75(8)
O6	Ca2	Ca1	40.90(5)	O11	Ca1	O6	72.24(8)
O6	Ca2	O8[1]	155.12(7)	O11	Ca1	O1[3]	78.82(9)
O6	Ca2	O4	75.34(7)	O11	Ca1	O5	120.20(8)
O6	Ca2	O7	77.70(7)	O11	Ca1	C1[3]	102.00(9)
O6	Ca2	O7[1]	150.95(7)	O12	Ca1	Ca2	115.31(7)
O6	Ca2	O3	100.15(7)	O12	Ca1	Ca1[2]	85.48(8)
O6	Ca2	O9	82.88(7)	O12	Ca1	O4	83.54(8)
O6	Ca2	O10	89.15(8)	O12	Ca1	O2[3]	92.28(8)
O6	Ca2	C10[1]	171.46(8)	O12	Ca1	O2[4]	80.30(9)
O7[1]	Ca2	Ca2[1]	36.03(5)	O12	Ca1	O6	142.73(9)
O7	Ca2	Ca2[1]	37.56(5)	O12	Ca1	O1[3]	114.16(9)
O7	Ca2	Ca1	99.64(5)	O12	Ca1	O5	160.04(9)

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
O7^{1}	Ca2	Ca1	149.79(5)	O12	Ca1	O11	79.17(10)
O7^{1}	Ca2	O8^{1}	52.83(7)	O12	Ca1	C1^{3}	107.52(9)
O7	Ca2	O8^{1}	122.99(7)	C1^{3}	Ca1	Ca2	136.17(6)
O7	Ca2	O4	117.51(7)	C1^{3}	Ca1	Ca1^{2}	60.65(6)
O7	Ca2	O7^{1}	73.59(8)	C10	O8	Ca2^{1}	91.77(16)
O7	Ca2	O3	79.72(7)	Ca1	O4	Ca2	110.08(8)
O7^{1}	Ca2	O3	79.15(7)	C5	O4	Ca2	94.27(16)
O7	Ca2	O9	148.86(7)	C5	O4	Ca1	119.16(17)
O7	Ca2	O10	79.36(8)	Ca1^{4}	O2	Ca1^{5}	105.03(7)
O7	Ca2	C10^{1}	97.53(7)	C1	O2	Ca1^{4}	147.28(19)
O7^{1}	Ca2	C10^{1}	26.59(7)	C1	O2	Ca1^{5}	93.89(17)
O3	Ca2	Ca2^{1}	76.76(5)	Ca2	O6	Ca1	103.15(7)
O3	Ca2	Ca1	70.65(5)	C6	O6	Ca2	115.10(17)
O3	Ca2	C10^{1}	71.85(7)	C6	O6	Ca1	86.41(16)
O9	Ca2	Ca2^{1}	148.15(6)	Ca2	O7	Ca2^{1}	106.41(7)
O9	Ca2	Ca1	80.42(6)	C10	O7	Ca2	147.59(18)
O9	Ca2	O8^{1}	82.97(7)	C10	O7	Ca2^{1}	92.51(16)
O9	Ca2	O4	79.94(8)	C5	O3	Ca2	87.17(17)
O9	Ca2	O7^{1}	120.72(8)	C1	O1	Ca1^{5}	91.17(16)
O9	Ca2	O3	128.02(7)	C6	O5	Ca1	96.73(18)
O9	Ca2	O10	76.22(8)	C11	O12	Ca1	152.0(3)
O9	Ca2	C10^{1}	104.31(8)	O2	C1	Ca1^{5}	60.34(14)
O10	Ca2	Ca2^{1}	77.97(6)	O4	Ca1	Ca2	35.43(5)
O10	Ca2	Ca1	127.09(7)	O4	Ca1	Ca1^{2}	115.32(5)
O10	Ca2	O8^{1}	107.14(9)	O4	Ca1	O2^{3}	152.03(7)
O10	Ca2	O4	152.97(8)	O4	Ca1	O2^{4}	77.07(7)
O10	Ca2	O7^{1}	81.39(8)	O4	Ca1	O6	71.33(7)
O10	Ca2	O3	154.69(8)	O4	Ca1	O1^{3}	153.68(7)
O10	Ca2	C10^{1}	96.99(9)	O4	Ca1	O5	92.54(7)
C10^{1}	Ca2	Ca2^{1}	60.80(6)	O4	Ca1	O11	86.13(9)
C10^{1}	Ca2	Ca1	134.84(6)	O4	Ca1	C1^{3}	167.21(8)
Ca1^{2}	Ca1	Ca2	129.76(3)	O2^{4}	Ca1	Ca2	97.74(5)
O2^{3}	Ca1	Ca2	150.19(5)	O2^{4}	Ca1	C1^{3}	98.09(8)
O2^{3}	Ca1	Ca1^{2}	36.72(5)	O2^{3}	Ca1	C1^{3}	25.77(7)
O2^{4}	Ca1	Ca1^{2}	38.25(5)	O6	Ca1	Ca2	35.95(4)
O2^{4}	Ca1	O2^{3}	74.97(7)	O6	Ca1	Ca1^{2}	129.85(5)
O2^{3}	Ca1	O6	122.64(6)	O6	Ca1	C1^{3}	101.51(7)
O2^{4}	Ca1	O6	118.47(7)	O1^{3}	Ca1	Ca2	119.27(6)
O2^{3}	Ca1	O1^{3}	51.26(7)	O1^{3}	Ca1	Ca1^{2}	86.54(5)
O2^{4}	Ca1	O1^{3}	123.41(7)	C8	C10	Ca2^{1}	170.81(18)

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
O2[4]	Ca1	O5	79.75(7)	O7	C10	Ca2[1]	60.90(14)

Symmetry transformations used to generate equivalent atoms: [1]2-X,1-Y,1-Z; [2]1-X,-Y,-Z; [3]+X,-1+Y,+Z; [4]1-X,1-Y,-Z; [5]+X,1+Y,+Z.

Table S8. Bond Lengths (Å) for **Ca-MOF 4**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Ca2	Ca1[1]	3.606(11)	Ca2	O10	2.438(11)
Ca2	Ca1	3.607(10)	Ca1	O6[2]	2.569(15)
Ca2	O6[2]	2.344(14)	Ca1	O12[2]	2.337(13)
Ca2	O12	2.548(14)	Ca1	O13	2.347(14)
Ca2	O13	2.455(14)	Ca1	O5[2]	2.464(13)
Ca2	O5	2.344(13)	Ca1	O14	2.579(13)
Ca2	O11	2.408(11)	Ca1	O9[2]	2.539(13)
Ca2	O14	2.552(13)	Ca1	O15	2.405(11)
Ca2	O9	2.581(14)	Ca1	O16	2.439(10)

Symmetry transformations used to generate equivalent atoms: [1]1+X,+Y,+Z; [2]-1+X,+Y,+Z.

Table S9. Bond Angles (°) for **Ca-MOF 4**.

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
Ca1[1]	Ca2	Ca1	129.6(2)	O15	Ca1	Ca2[2]	111.3(4)
O6[2]	Ca2	Ca1	45.3(3)	O15	Ca1	Ca2	108.7(4)
O6[2]	Ca2	Ca1[1]	169.4(3)	O15	Ca1	O6[2]	142.6(4)
O6[2]	Ca2	O12	131.7(4)	O15	Ca1	O5[2]	149.1(4)
O6[2]	Ca2	O13	80.1(4)	O15	Ca1	O14	77.1(4)
O6[2]	Ca2	O11	80.8(5)	O15	Ca1	O9[2]	81.7(4)
O6[2]	Ca2	O14	69.3(5)	O15	Ca1	O16	111.9(4)
O6[2]	Ca2	O9	144.1(4)	O15	Ca1	C13[2]	154.9(3)
O6[2]	Ca2	O10	75.2(5)	O16	Ca1	Ca2	97.4(3)
O12	Ca2	Ca1	90.1(4)	O16	Ca1	Ca2[2]	94.9(4)
O12	Ca2	Ca1[1]	40.2(3)	O16	Ca1	O6[2]	95.8(4)
O12	Ca2	O14	93.6(4)	O16	Ca1	O5[2]	86.7(4)
O12	Ca2	O9	65.3(4)	O16	Ca1	O14	140.0(4)
O13	Ca2	Ca1[1]	92.0(3)	O16	Ca1	O9[2]	139.5(4)
O13	Ca2	Ca1	40.2(3)	O16	Ca1	C13[2]	93.2(4)

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
O13	Ca2	O12	51.8(4)	C13^{2}	Ca1	Ca2	67.3(4)
O13	Ca2	O14	68.5(4)	C13^{2}	Ca1	Ca2^{2}	63.4(4)
O13	Ca2	O9	104.5(4)	Ca2^{1}	O6	Ca1^{1}	94.4(4)
O5	Ca2	Ca1	160.5(3)	C13	O6	Ca2^{1}	175.7(10)
O5	Ca2	Ca1^{1}	42.7(3)	C13	O6	Ca1^{1}	89.9(9)
O5	Ca2	O6^{2}	137.7(4)	Ca1^{1}	O12	Ca2	95.0(5)
O5	Ca2	O12	77.6(4)	C12	O12	Ca2	91.5(10)
O5	Ca2	O13	122.8(4)	C12	O12	Ca1^{1}	173.4(11)
O5	Ca2	O11	87.9(4)	Ca1	O13	Ca2	97.3(4)
O5	Ca2	O14	148.8(4)	C12	O13	Ca2	95.4(9)
O5	Ca2	O9	69.8(4)	C12	O13	Ca1	152.3(10)
O5	Ca2	O10	71.4(5)	Ca2	O5	Ca1^{1}	97.1(5)
O11	Ca2	Ca1	110.6(4)	C13	O5	Ca2	150.4(10)
O11	Ca2	Ca1^{1}	109.3(4)	C13	O5	Ca1^{1}	96.7(9)
O11	Ca2	O12	143.0(4)	Ca2	O14	Ca1	89.3(4)
O11	Ca2	O13	148.4(4)	Ca1^{1}	O9	Ca2	89.5(4)
O11	Ca2	O14	81.3(4)	O13	Ca1	O6^{2}	77.7(4)
O11	Ca2	O9	77.7(4)	O13	Ca1	O5^{2}	122.8(4)
O11	Ca2	O10	111.3(4)	O13	Ca1	O14	69.6(4)
O14	Ca2	Ca1	45.6(3)	O13	Ca1	O9^{2}	148.5(4)
O14	Ca2	Ca1^{1}	114.5(3)	O13	Ca1	O15	87.2(5)
O14	Ca2	O9	79.3(3)	O13	Ca1	O16	71.9(5)
O9	Ca2	Ca1	118.8(3)	O13	Ca1	C13^{2}	102.3(5)
O9	Ca2	Ca1^{1}	44.8(3)	O5^{2}	Ca1	Ca2^{2}	40.2(3)
O10	Ca2	Ca1^{1}	97.6(4)	O5^{2}	Ca1	Ca2	92.1(4)
O10	Ca2	Ca1	95.4(4)	O5^{2}	Ca1	O6^{2}	51.8(3)
O10	Ca2	O12	96.2(4)	O5^{2}	Ca1	O14	104.9(4)
O10	Ca2	O13	87.6(4)	O5^{2}	Ca1	O9^{2}	68.8(4)
O10	Ca2	O14	139.8(4)	O5^{2}	Ca1	C13^{2}	25.1(4)
O10	Ca2	O9	139.7(4)	O14	Ca1	Ca2	45.0(3)
Ca2^{2}	Ca1	Ca2	129.6(2)	O14	Ca1	Ca2^{2}	118.8(3)
O6^{2}	Ca1	Ca2^{2}	89.9(3)	O14	Ca1	C13^{2}	84.5(4)
O6^{2}	Ca1	Ca2	40.4(3)	O9^{2}	Ca1	Ca2^{2}	45.7(3)
O6^{2}	Ca1	O14	65.6(4)	O9^{2}	Ca1	Ca2	114.6(3)
O6^{2}	Ca1	C13^{2}	26.9(4)	O9^{2}	Ca1	O6^{2}	93.5(4)
O12^{2}	Ca1	Ca2^{2}	44.7(4)	O9^{2}	Ca1	O14	79.2(3)
O12^{2}	Ca1	Ca2	169.0(3)	O9^{2}	Ca1	C13^{2}	78.2(4)
O12^{2}	Ca1	O6^{2}	131.0(4)	O12^{2}	Ca1	C13^{2}	104.5(5)
O12^{2}	Ca1	O13	138.3(4)	O13	Ca1	Ca2	42.5(3)
O12^{2}	Ca1	O5^{2}	79.4(5)	O13	Ca1	Ca2^{2}	160.6(3)

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
O12[2]	Ca1	O14	144.0(4)	O12[2]	Ca1	O15	81.9(5)
O12[2]	Ca1	O9[2]	69.0(4)	O12[2]	Ca1	O16	75.3(5)

Symmetry transformations used to generate equivalent atoms: [1]1+X,+Y,+Z; [2]-1+X,+Y,+Z.

Table S10. Hydrogen bonds for **Ca-MOF-4** (Å) and (°).

D-H···A	d(D-H)	d(H···A)	d(D···A)	∟(DHA)	Symmetry Code
O9-H9A···O7	0.99	1.76	2.702(19)	159	x,1+y,-1+z
O9-H9B···O2	0.99	1.74	2.697(18)	161	x,y,1+z
O10-H10A···O1	0.87	2.19	2.812(18)	128	-1+x,-1+y,1+z
O10-H10A···O6	0.87	2.50	2.912(18)	110	-1+x,y,z
O11-H11A···O2	0.88	1.91	2.739(19)	155	x,y,1+z
O11-H11B···O1	0.89	1.99	2.771(19)	147	-1+x,y,1+z
O14-H14A···O8	0.99	1.76	2.722(18)	162	1+x,1+y,-1+z
O14-H14B···O1	0.99	1.77	2.714(19)	159	x,y,1+z
O15-H15A···O8	0.87	1.92	2.753(19)	160	1+x,1+y,-1+z
O15-H15B···O7	0.88	1.91	2.76(2)	164	x,1+y,-1+z
O16-H16A···O7	0.87	2.05	2.777(19)	140	x,y,-1+z
O16-H16B···O8	0.87	2.32	3.134(19)	156	1+x,y,-1+z

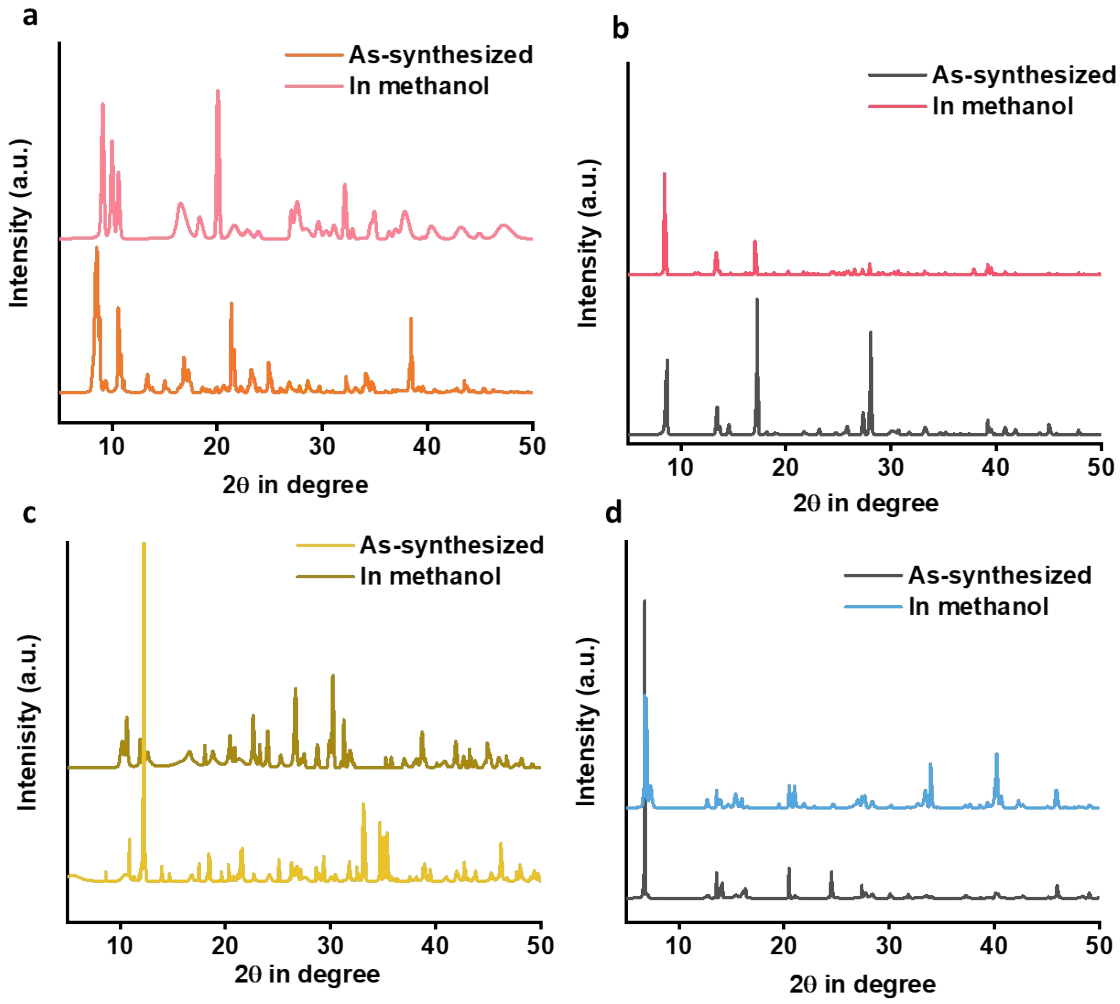


Figure S5. PXRD pattern of Ca-MOF-1 (a), Ca-MOF-2 (b), Ca-MOF-3 (c) and Ca-MOF-4 (d) in methanol.

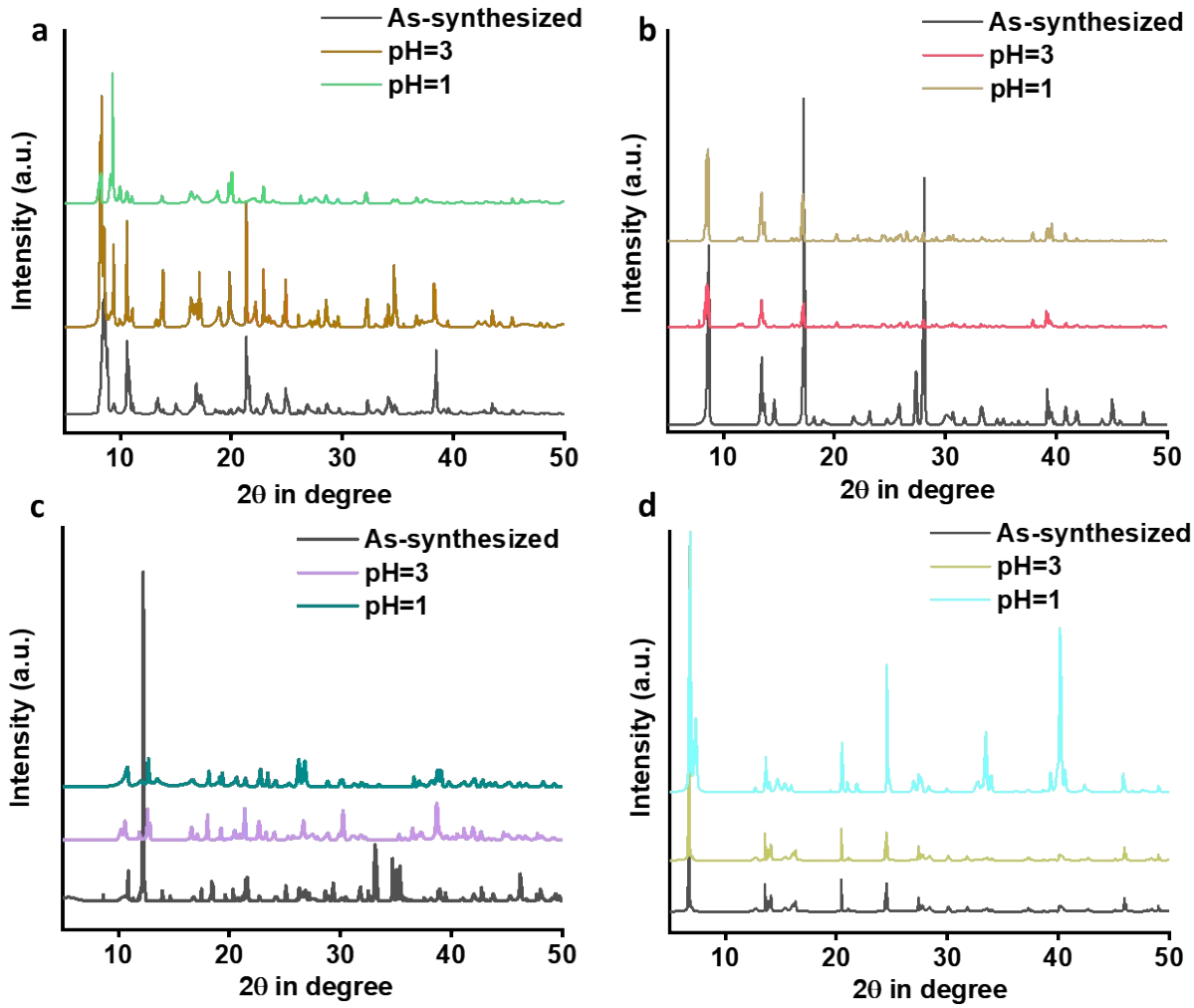


Figure S6. PXRD pattern of Ca-MOF-1 (a), Ca-MOF-2 (b), Ca-MOF-3 (c) and Ca-MOF-4 (d) at different pH medium.

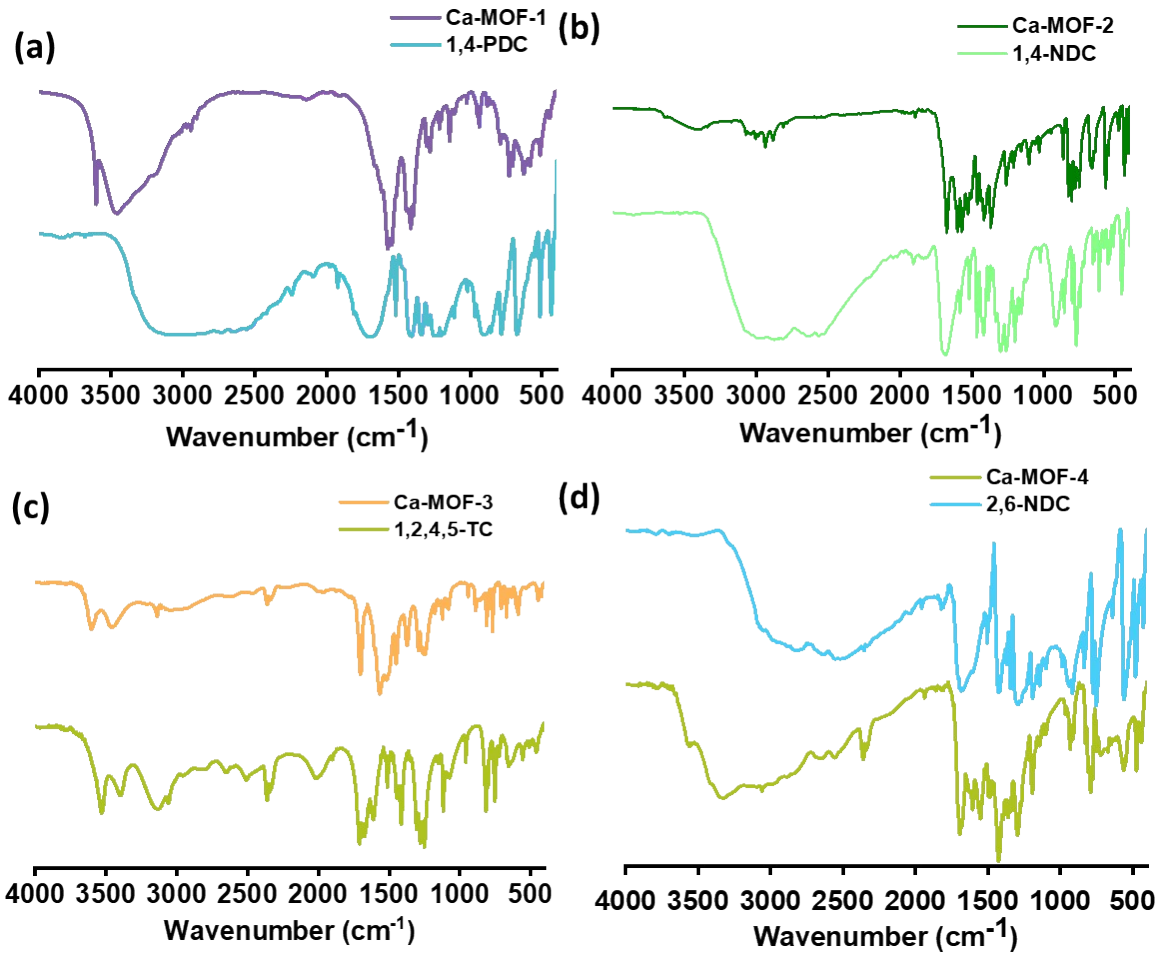


Figure S7. FT-IR of Ca-MOF-1 (a), Ca-MOF-2 (b), Ca-MOF-3 (c) and Ca-MOF-4 (d).

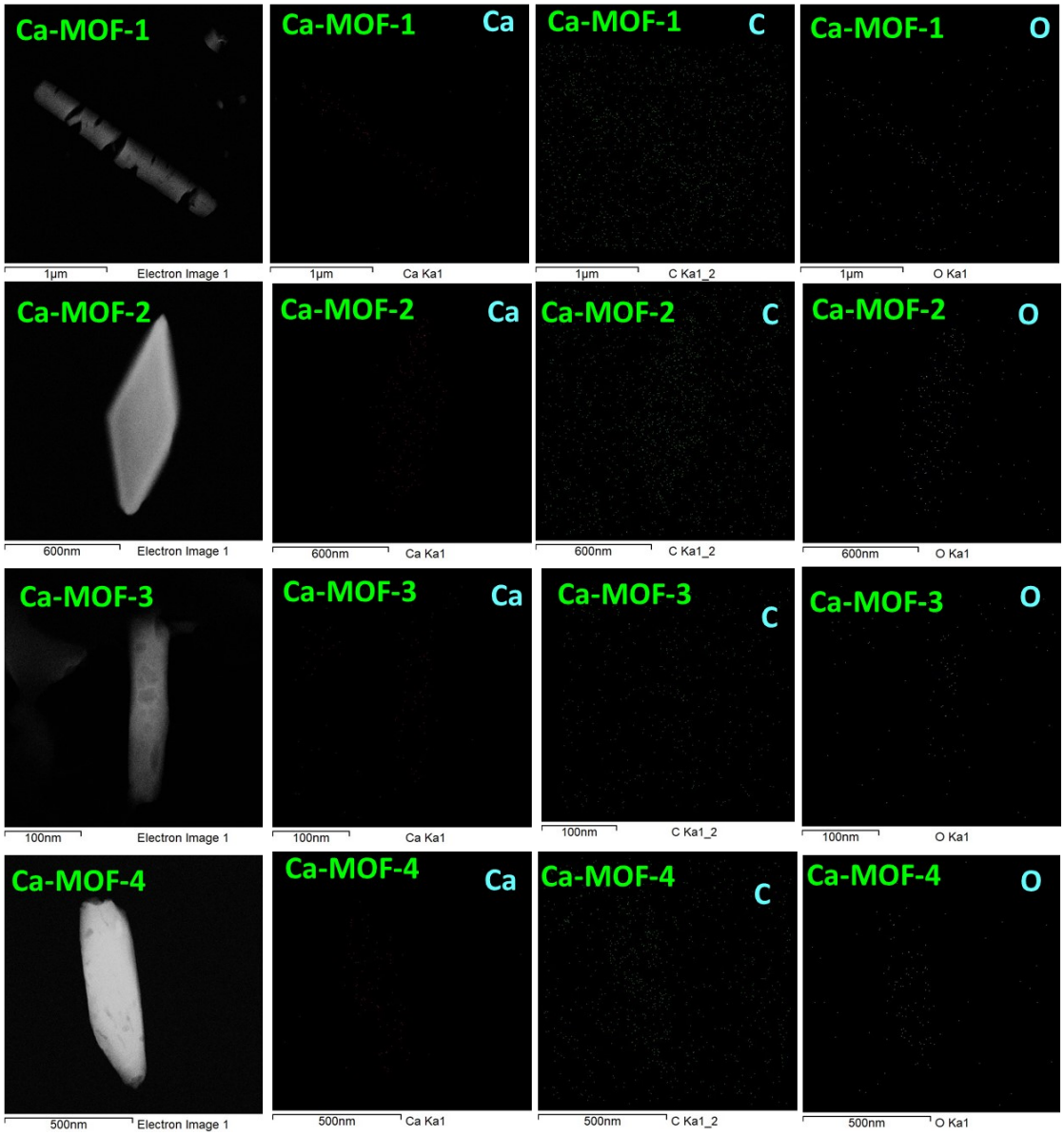


Figure S8. Elemental mapping of Ca-MOFs.

Thermo-gravimetric analysis

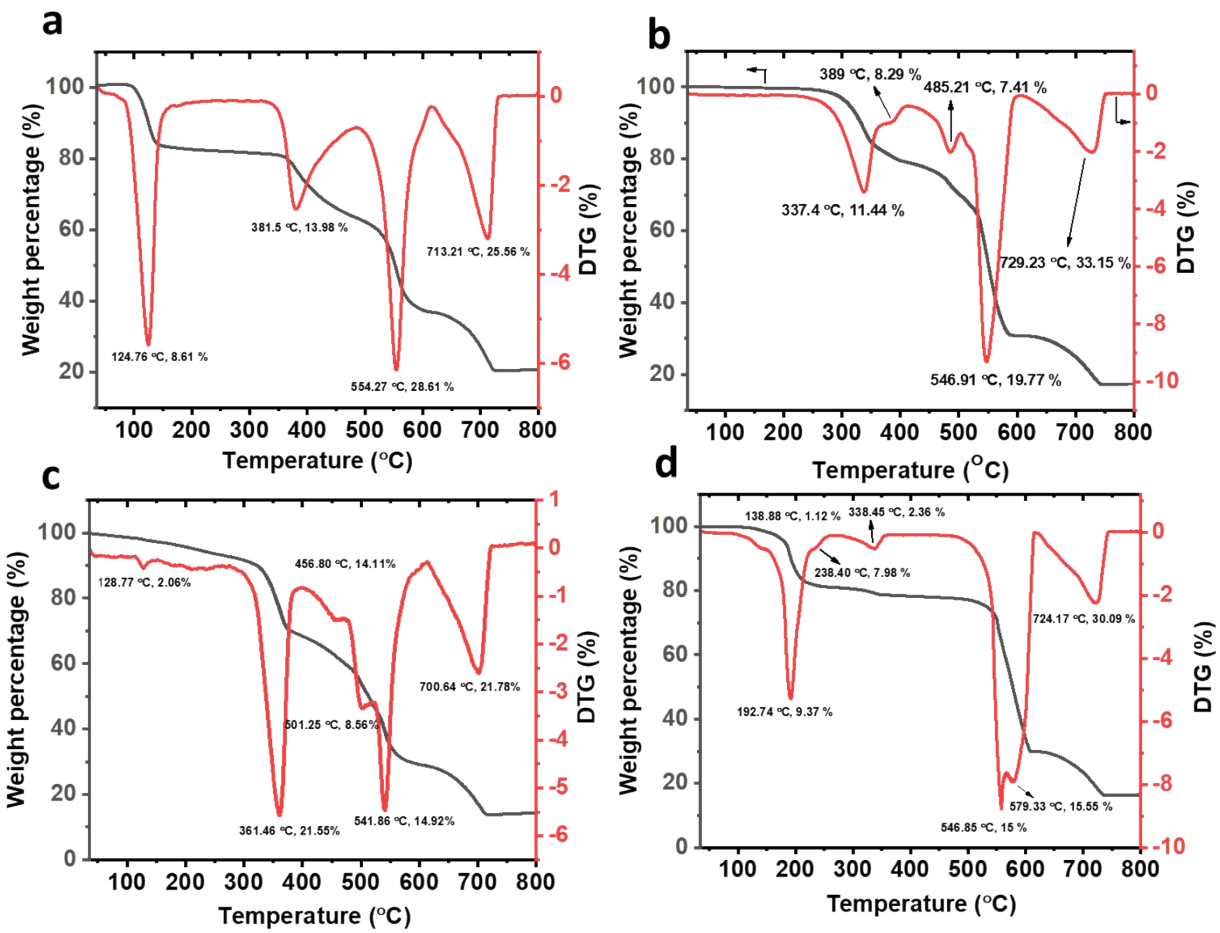


Figure S9. TGA and DTG plot of Ca-MOF-1 (a), Ca-MOF-2 (b), Ca-MOF-3 (c) and Ca-MOF-4 (d).

QTAIM Analysis:

QTAIM analysis is the topological analysis of atoms in a molecule. This formalism is employed by AIMAll program, where the classical definition of a 'bond' is considered to be the 'bond path', indicating a line of maximum electron density linking the bonded pairs of atoms in an equilibrium geometry. The interaction of two atoms at a certain distance creates a critical point (Bond Critical Point-BCP) in the electron density [ρ(r)] where the gradient $\nabla\rho(r)$ vanishes. The strength of this interaction in varied molecular systems largely depends upon two important parameters, viz., electron density and its Laplacian [$\nabla^2\rho(r)$] at the concerned BCP.

Electronic energy density [H(r)] is defined as

$H(r) = G(r) + V(r)$

Where H(r), G(r) and V(r) are the electronic, kinetic and potential energy densities, respectively. The ratio [-G(r)/V(r)] predicts the nature of the bonding interaction. [-G(r)/V(r)]>1 indicates non-covalent interaction whereas 0.5 < [-G(r)/V(r)] < 1 specifies partly covalent interaction. Negative values of both $\nabla^2\rho(r)$ and H(r) indicate the interaction to be strong, for medium interaction H(r) is negative but $\nabla^2\rho(r)$ is positive, and the interactions are weak when both are positive.

Table S11: AIM analysis of **EM-2** concerning the epoxide binding with the metal centre, at B3LYP/6-31G (d,p) level.

System	BCP	ρ(r)	$\nabla^2\rho(r)$	G	V	H	-G/V
EM-2	O74-Ca22	0.025	0.120	0.027	-0.024	0.003	1.121

Chromatography data

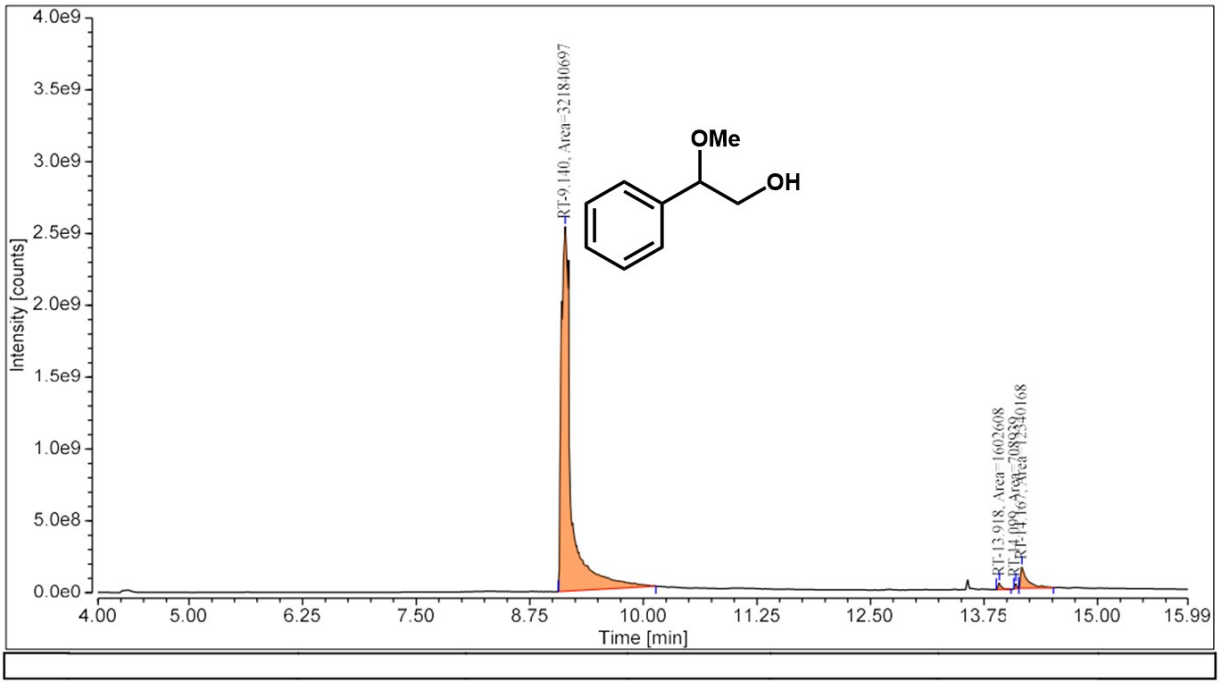


Figure S10: GC analysis of styrene oxide conversion under standard conditions.

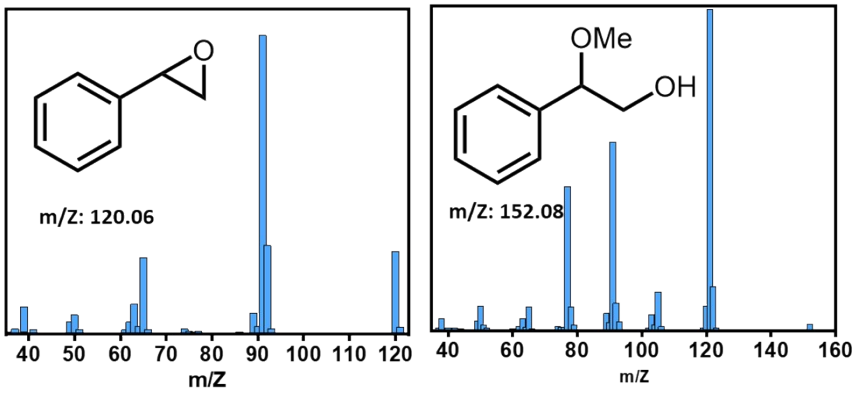


Figure S11: Mass fragmentation of styrene oxide and the reaction product.

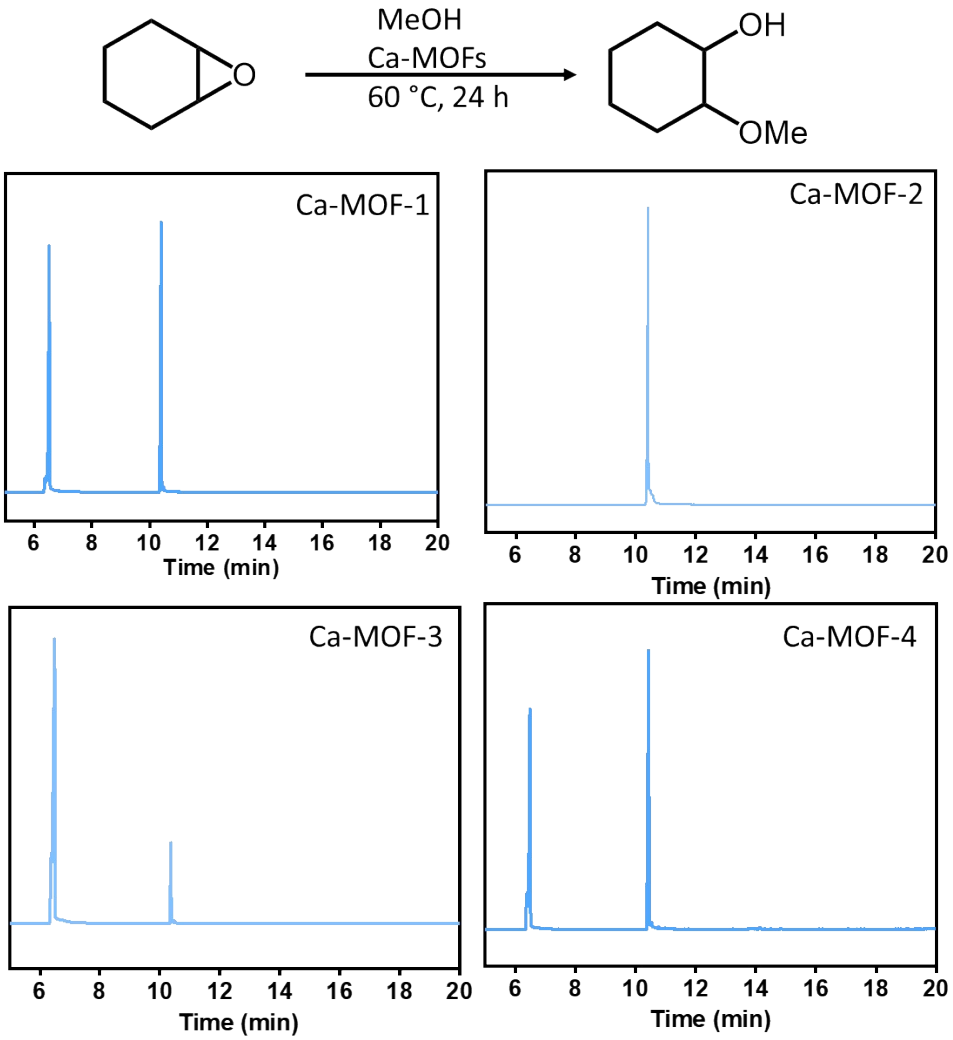


Figure S12: GC analysis of cyclohexane oxide using over different Ca-MOFs.

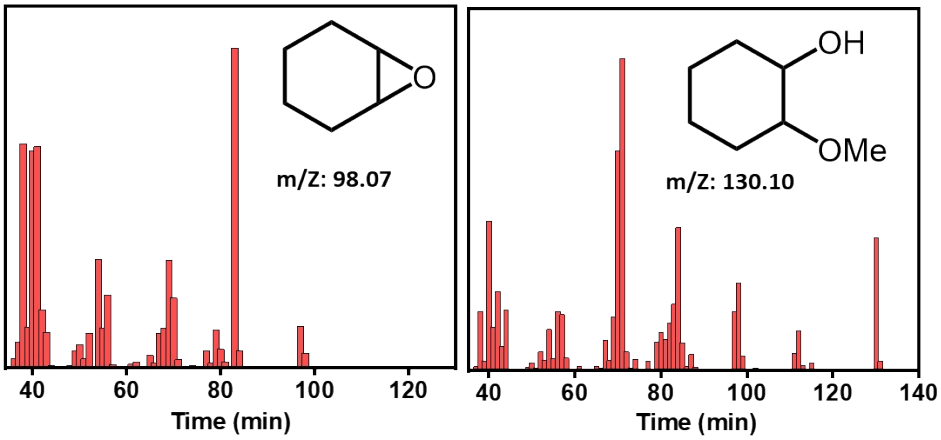


Figure S13: Mass fragmentation of cyclohexane oxide and the reaction product.

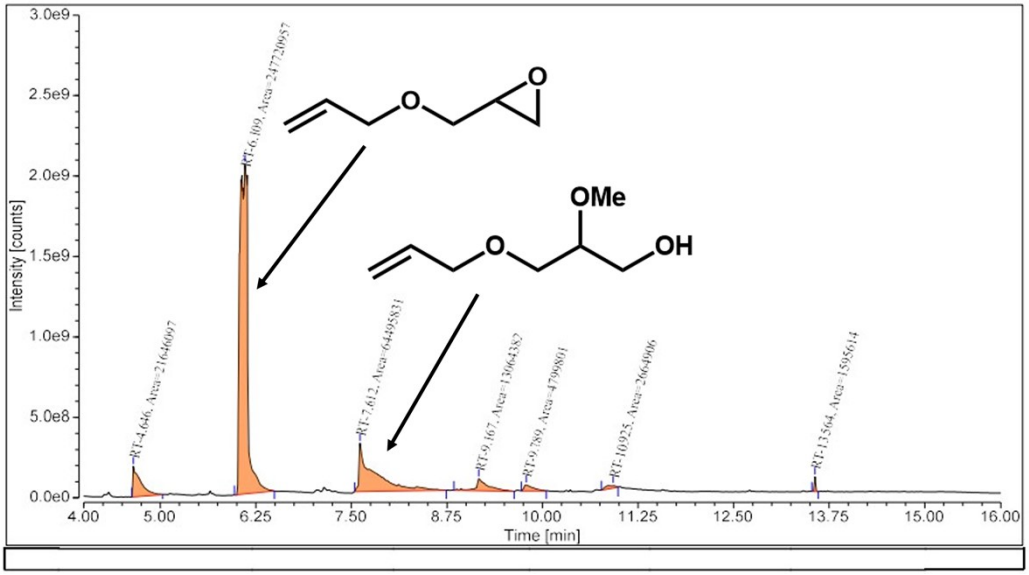


Figure S14: GC analysis for the allyl-glycidyl ether conversion.

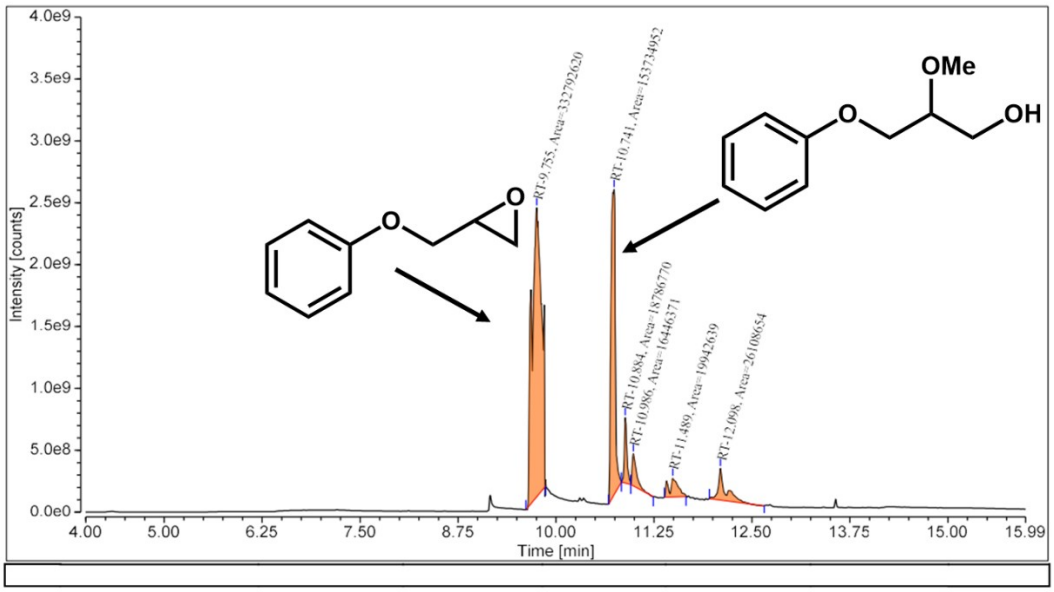


Figure S15: GC analysis for the phenyl glycidyl ether conversion.

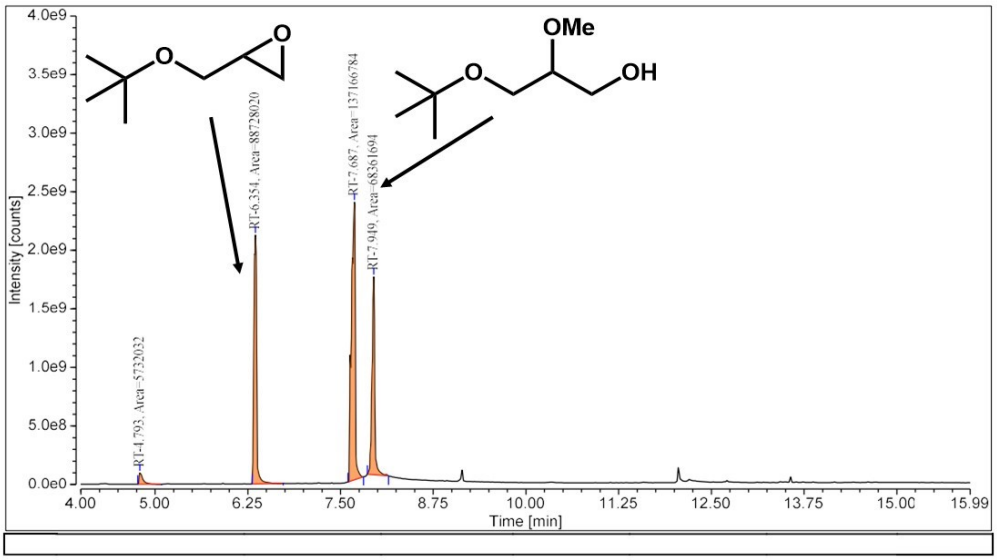


Figure S16: GC analysis of the reaction mixture for tertiary butyl-glycidyl ether.

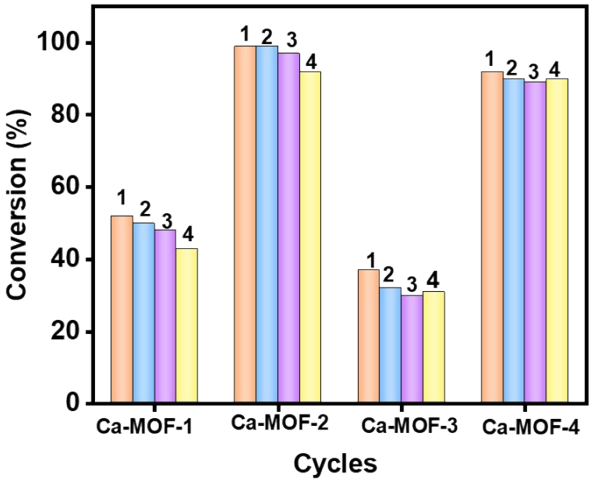


Figure S17: Recyclablity of Ca-MOFs for consecutive four reaction cycles in the methanolysis of styrene oxide.

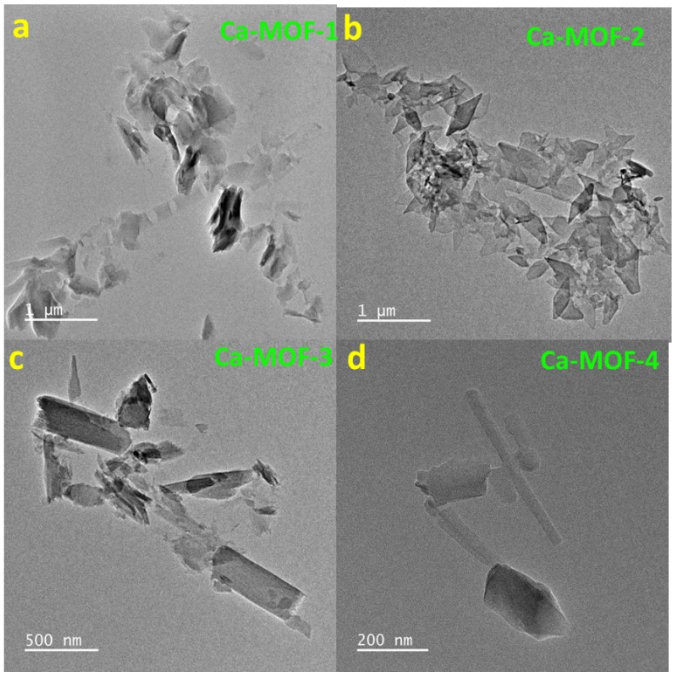


Figure S18. TEM images of Ca-MOFs after catalysis.

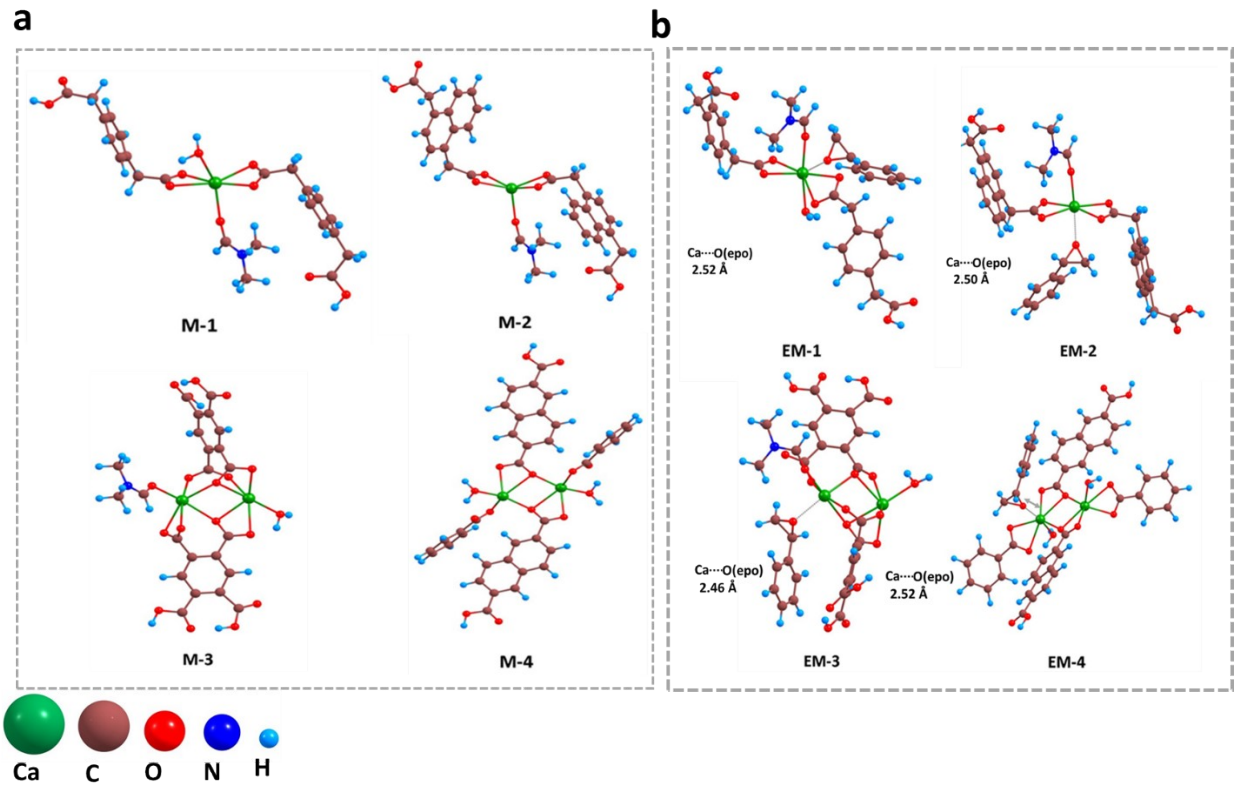
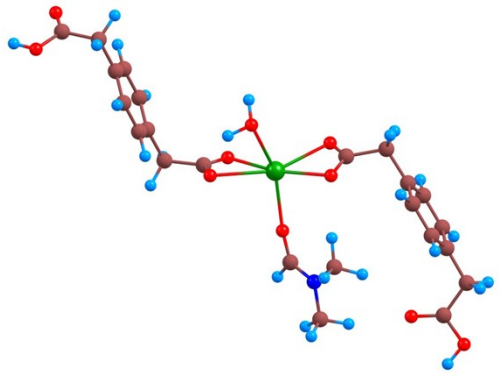


Figure S19. DFT optimized structures of the model MOF structures (a) and corresponding epoxide bonded complexes (b).

Cartesian Co-ordinates

M-1



0 1

C	-5.31392800	1.05589300	-0.79938300
C	-5.05694100	1.12306500	0.57700000
C	-5.91476500	0.43546100	1.44520400
C	-6.99692100	-0.29584200	0.95748600
C	-7.24962900	-0.36173500	-0.41791100
C	-6.39655200	0.32567200	-1.28826500
H	-4.65279500	1.57403400	-1.48689900
H	-5.73385200	0.47462200	2.51607900
H	-7.65905900	-0.81127200	1.64749500
H	-6.58154600	0.29230500	-2.35898100
C	-8.43218100	-1.15941500	-0.94810700
H	-8.41639900	-1.17724500	-2.04021100
H	-8.39554100	-2.18835800	-0.57839300
C	-3.86872100	1.89935900	1.11141900
H	-3.82611900	2.88569700	0.63594400
C	-9.74514500	-0.56844500	-0.46941700
O	-10.28974800	-0.83238700	0.58013000
O	-10.24248600	0.33884900	-1.34353000
H	-11.04959000	0.69319400	-0.93263700
C	-2.54661200	1.18471300	0.80827400
O	-2.16769700	1.12812100	-0.41378100
O	-1.89917300	0.66046000	1.75593800
H	-3.95356300	2.03432200	2.19128200
Ca	-0.16996400	-0.18574000	0.29730400
C	5.04631900	-2.17616700	1.26975700
C	4.27620700	-2.51195800	0.14915800
C	4.78735000	-2.20811900	-1.11953500
C	6.02612800	-1.58559100	-1.26075600
C	6.78893300	-1.24042900	-0.13882600
C	6.28361000	-1.54942600	1.12833100
H	4.67263100	-2.41004500	2.26310900
H	4.20292100	-2.45644300	-1.99998800

H	6.40517600	-1.36597700	-2.25618700
H	6.86300200	-1.30105700	2.01451600
C	8.12089100	-0.54661700	-0.28698600
H	8.81377000	-0.82729700	0.51372700
H	8.61838000	-0.83518900	-1.22170100
C	2.91418200	-3.14865000	0.31221600
H	2.85073500	-3.69918700	1.25286300
H	2.72824100	-3.84723000	-0.51134200
C	1.78645300	-2.10309400	0.28441100
O	1.65213400	-1.39553300	-0.76321900
O	1.04333900	-1.98895600	1.30581900
C	8.03736300	0.97116800	-0.29770600
O	7.03282100	1.64547600	-0.38294800
O	9.27082300	1.52250400	-0.21516600
H	9.14493200	2.48580500	-0.25045600
O	-1.88510300	-1.47380400	-0.95631700
H	-2.45955900	-2.15790000	-0.59242200
H	-2.41799200	-0.65247100	-1.00836800
C	2.14453100	2.52505400	0.49660400
O	1.26327200	1.65294300	0.48151400
N	3.26209800	2.51831000	-0.23472300
H	2.05059400	3.40314000	1.15406100
C	4.20794000	3.62746000	-0.17962700
H	3.90710200	4.33391600	0.59734000
H	5.21072700	3.24997400	0.03525400
H	4.23306800	4.15389400	-1.14113600
C	3.57136200	1.42551400	-1.15938600
H	2.91952700	0.57388500	-0.96513200
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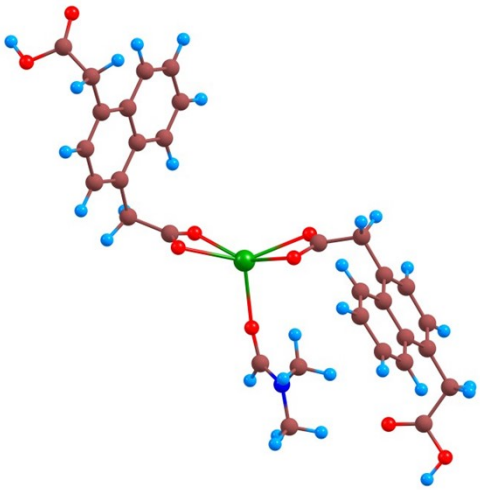
H	4.61322900	1.13036900	-1.01835400

M-2



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C	6.45428900	-0.46973000	-0.20536200
C	6.93073100	-0.41032900	1.14527500
C	6.45637900	0.57773500	1.97980000
H	5.17431400	2.29722500	2.22345700
H	6.81202800	0.62856900	3.00539600
C	7.92984000	-1.42529400	1.67483500
H	7.97194100	-1.34070800	2.76510700
H	7.63542200	-2.44743000	1.42609900
C	4.02584900	2.56208700	-0.19700200
H	3.99277700	3.35236800	0.55922300
C	9.34181200	-1.23210400	1.14663000
O	9.92883900	-1.98683200	0.40164500
O	9.90173400	-0.09114700	1.61368500
H	10.78453600	-0.04121800	1.20958800
C	2.59919800	2.01760300	-0.34055000
O	2.00252500	1.60600800	0.70293500
O	2.06654100	1.99070300	-1.49749900
H	4.32034300	3.01385600	-1.14762600
Ca	0.12101900	0.95043200	-0.59267500
C	-4.46951500	-1.77764500	-2.04525200
C	-3.73365300	-2.13300400	-0.93304000
C	-4.36579100	-2.09581800	0.35496400
C	-5.74938600	-1.71317800	0.45542000
C	-6.46369900	-1.33063700	-0.72536000
C	-5.81683100	-1.37312900	-1.94091400
H	-3.99977300	-1.80606000	-3.02413500
H	-6.35241100	-1.09093300	-2.84393100
C	-7.90172100	-0.87864400	-0.65913400
H	-8.33406000	-0.85480700	-1.66672700
H	-8.53585700	-1.56618500	-0.08857000
C	-2.27952500	-2.52628700	-1.11313600
H	-2.12886200	-2.90351400	-2.12602700
H	-1.99251500	-3.31125900	-0.40828000
C	-1.34624500	-1.32384800	-0.91383800
O	-1.13179200	-0.91109200	0.27254600
O	-0.85027200	-0.76794800	-1.94004700
C	-8.09622200	0.51543200	-0.08452000
O	-7.23327000	1.34079100	0.12809900
O	-9.40562600	0.76217700	0.15186100
H	-9.45937000	1.67368000	0.48567300
C	-2.59729900	3.19114100	-0.19426300
O	-1.57111600	2.51202900	-0.36994500

N	-3.66390600	2.82223900	0.51492700
H	-2.68504400	4.19145600	-0.64298400
C	-4.80636000	3.71606200	0.68328100
H	-4.66050800	4.62037700	0.08856100
H	-5.72132000	3.21039600	0.36507500
H	-4.90953400	4.00107400	1.73651600
C	-3.74251000	1.52062200	1.18132200
H	-2.91615400	0.88585200	0.86559100
H	-3.69860700	1.65654700	2.26761000
H	-4.69078100	1.04629500	0.92001300
C	4.99280700	0.39386200	-1.98592700
C	6.90884400	-1.45660400	-1.12406800
C	5.44927100	-0.58332400	-2.84305000
C	6.42014200	-1.51196900	-2.41057500
H	4.23083500	1.08760200	-2.32350300
H	5.06038300	-0.63829400	-3.85577000
H	6.78411900	-2.27369100	-3.09403300
H	7.66834400	-2.16582600	-0.81476000
C	-6.36156900	-1.71150500	1.73989700
C	-3.66526000	-2.42086200	1.55016600
C	-5.65740900	-2.05601700	2.87138600
H	-2.60703800	-2.64130800	1.49470600
C	-4.29255300	-2.40507400	2.77580600
H	-3.73408900	-2.65660600	3.67248300
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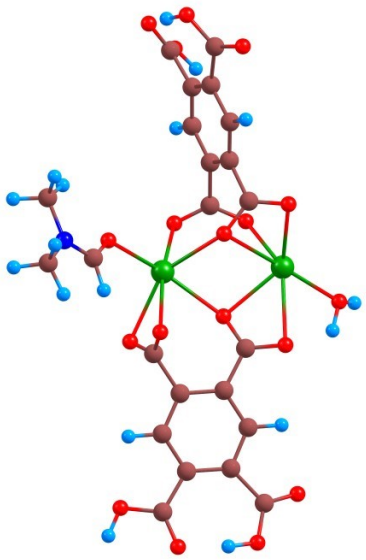
M-3



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O	-7.91405300	0.50297800	1.44297900
O	1.39318200	-1.01982300	0.40477300
O	1.78850600	1.72172800	-0.60991000
O	-1.61615300	-0.31241100	2.08485700
O	-7.10935600	-1.03110500	2.80499800
O	2.40581100	-2.47254900	-0.92667900
O	1.13158300	-4.77410300	-0.25256200
H	1.19602100	-5.57162400	0.28441800
H	2.02924800	-4.41975500	-0.39091700
C	-7.04064800	-0.31799600	1.66609000
C	2.44282900	1.47609600	0.44926100
C	-2.11206900	-1.28128100	1.44950600
C	3.73844500	0.71080000	0.28513200
C	3.71797900	-0.64918000	-0.07804000
C	-3.45188700	-1.04142800	0.76896600
C	-5.84739100	-0.56478700	0.79182600
C	-4.63445700	-0.81812200	1.46156800
H	-4.59965500	-0.79463000	2.54715600
C	2.43663600	-1.42213400	-0.21858900
C	4.97114800	1.32799100	0.46430600
H	4.99594600	2.36765100	0.76448100
O	7.08951600	-2.90085200	-0.31602700
O	8.53907800	1.22407800	0.00933000
O	8.54930100	-1.26534400	-0.59541600
O	7.21543400	2.59716000	1.15060900
C	7.32481600	-1.70901500	-0.34038800
C	6.17393700	-0.71881800	-0.11807800
C	6.18874300	0.65279900	0.26046800
C	7.41996600	1.47104200	0.44746000
C	4.92097000	-1.32486200	-0.26903300
H	4.90338300	-2.37411900	-0.53247700
O	-8.09195200	0.42838700	-1.13557400
O	-1.18214800	-0.50821600	-1.00807700
O	-7.00190600	-0.69623100	-2.70186600
O	-1.99394900	-2.34383100	-1.97029300
C	-2.15777700	-1.28387500	-1.31797800
C	-7.05153300	-0.28108700	-1.56268600
C	-5.86751000	-0.52428900	-0.62524900
C	-3.47646200	-1.01728300	-0.63845400
C	-4.67090700	-0.78850400	-1.30907900
H	-4.70811500	-0.80769800	-2.39205700
H	8.61395100	-0.28076200	-0.51383500
H	8.06997300	3.06026000	1.17729600
H	-6.43471800	-1.72608600	2.80669500

H	-8.01860700	0.66884000	-0.17908700
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O	-1.17661000	2.94378200	0.22369700
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C	-0.55669800	5.98719700	-1.60537900
H	0.44829800	5.63892000	-1.85037700
H	-1.10341300	6.16934500	-2.53687900
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C	-2.60949000	5.27766400	-0.38057500
H	-2.98033800	4.43937400	0.20653700
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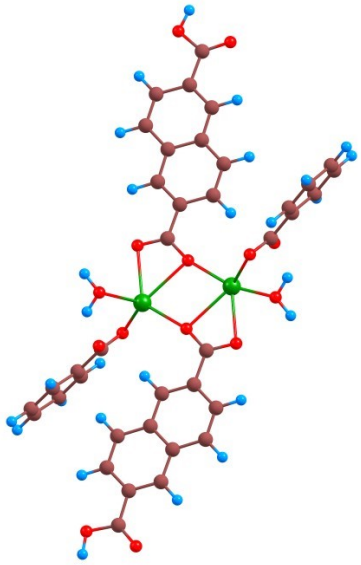
H	-3.24927600	5.42419700	-1.25710900

M-4



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O	1.33411400	-2.25901300	-0.67936700
C	-1.98888700	2.03284800	0.43762200
C	4.23409400	-0.29171800	0.43437400
C	3.46731800	-1.38018200	-0.06606600
C	-3.47591500	2.10276300	0.31600100
C	-5.62549700	1.08510600	-0.20205900
C	-4.21365500	1.01148500	-0.10289600

H	-3.72811200	0.07682000	-0.36316700
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H	6.18483000	0.43267600	0.91737000
C	5.50058000	-2.69633300	-0.33704700
C	6.27172100	-1.59620200	0.16370300
C	4.09621200	-2.55409700	-0.44119600
H	3.49455700	-3.37413200	-0.81877600
C	-6.28421300	2.31429400	0.12753600
C	-4.13309300	3.32134100	0.64642300
C	-5.49838100	3.42290900	0.55072700
H	-5.99944600	4.35437900	0.79905400
H	3.74700500	0.63092000	0.72925600
H	-3.52715100	4.15954600	0.96993200
C	7.67640600	-1.73730500	0.26569100
C	6.17068800	-3.89350900	-0.71360100
C	8.30038300	-2.91269900	-0.10821900
C	-6.40376700	-0.03053500	-0.61713100
C	-7.69358600	2.38103500	0.02243000
C	-7.77148300	0.06112500	-0.70827000
C	7.53515900	-4.00455500	-0.60424000
H	8.28174200	-0.91836200	0.64117700
H	8.04153600	-4.91810800	-0.89195000
H	5.58174000	-4.72460900	-1.09135900
C	9.77988500	-2.98599500	0.02840100
O	10.48759100	-2.09125300	0.44679200
O	10.28910700	-4.18013800	-0.36832400
H	11.24919300	-4.11328400	-0.23601100
C	-8.42637700	1.28207000	-0.38703200
H	-5.89203700	-0.95914500	-0.85277100
H	-8.36363400	-0.79032400	-1.02152700
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C	-9.90420800	1.42913700	-0.47266600
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O	-10.52632600	0.29550500	-0.88590300
H	-11.47409000	0.50806800	-0.90261400
C	4.21435000	4.44764700	-0.24533700
C	5.30898200	4.53116600	0.62482200
C	6.39235500	5.34886300	0.30968700
C	6.38699300	6.08842000	-0.87569400
C	5.29676100	6.00875000	-1.74596100
C	4.21320900	5.19071200	-1.43294300
H	5.29288100	3.94832700	1.53921300
H	7.24061200	5.41063600	0.98527100
H	7.23179700	6.72586200	-1.12109200
H	5.29344100	6.58414700	-2.66713700
H	3.35655700	5.11267500	-2.09312700

C	3.04848400	3.57004400	0.08913600
O	3.06015400	2.91637000	1.19380300
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C	-4.09918400	-3.92007700	0.37381000
C	-4.08642800	-4.66752000	1.55856500
C	-5.09918900	-5.58973300	1.81385100
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H	-3.27723800	-4.50983100	2.26286500
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H	-6.91579500	-6.49461000	1.08566700
H	-6.93841900	-5.18240600	-1.02271600
H	-5.12094400	-3.53086500	-1.47164700
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O	-3.07020800	-2.21236400	-0.96000800
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O	-1.21107600	-1.59518600	-2.80365600
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O	1.18312300	2.39529600	3.04754900
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Epoxide (E)

0 1

C	2.58788900	0.02112100	0.74351800
C	1.60256000	0.57915500	-0.20624400
O	2.48862900	-0.48157100	-0.59149700
H	3.49821600	0.57634400	0.97096200
H	2.23870800	-0.65267700	1.52551400
H	1.84077600	1.54428700	-0.65732500
C	0.14660500	0.26436300	-0.11790400
C	-0.78852700	1.30438300	-0.05885100
C	-0.30153300	-1.06176900	-0.07974200
C	-2.15031900	1.02489100	0.05541400
H	-0.44882600	2.33649000	-0.10213200
C	-1.66302300	-1.34004500	0.03040800
H	0.42617900	-1.86313500	-0.15887400
C	-2.59105400	-0.29867200	0.10209200
H	-2.86659500	1.84009300	0.10189400
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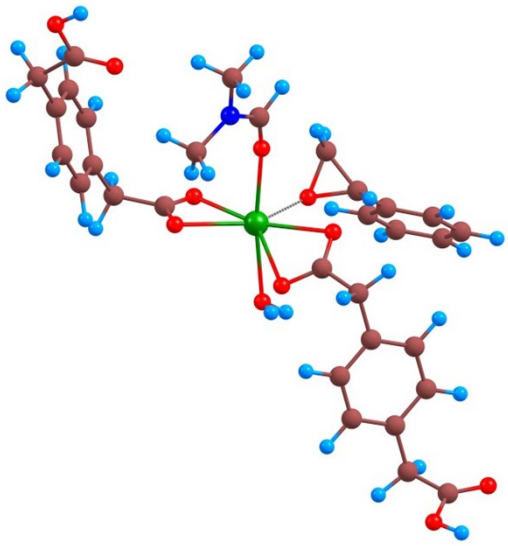
EM-1



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H	5.08042000	-0.72720300	2.24018900
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H	5.09840600	-3.70928300	-1.71136000
C	7.54947300	-2.54932700	-1.30006100
H	7.35899600	-3.16997500	-2.17846500
H	7.92585400	-1.57686400	-1.63130500
C	2.62593000	-1.85617000	1.81499900
H	2.18563900	-2.83229700	2.04924700
C	8.64454900	-3.17997100	-0.46064300
O	9.40398100	-2.57711600	0.26619000
O	8.66465300	-4.52880800	-0.58091100
H	9.35987300	-4.84199300	0.02273600
C	1.57258800	-1.05799500	1.03346100
O	1.06147300	-1.60247400	-0.00010200
O	1.26166500	0.10079800	1.42685700
H	2.83731400	-1.33739600	2.75225600
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C	-5.90202700	0.87645600	-1.97990600
C	-4.92521500	-0.01268900	-2.44433000
C	-5.11949300	-1.38311900	-2.22039900
C	-6.24890500	-1.84374900	-1.54786800
C	-7.21746000	-0.95113500	-1.07227000
C	-7.03121300	0.41512100	-1.30347700
H	-5.77649500	1.94254600	-2.15039100

H	-4.36764100	-2.08602800	-2.56368800
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H	-7.77519900	1.12719200	-0.95352600
C	-8.42813800	-1.44749400	-0.32096500
H	-9.29895200	-0.80344400	-0.48679600
H	-8.73032300	-2.44469200	-0.66533800
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H	-3.82698200	1.51023800	-3.50980000
H	-3.43218900	-0.15131700	-3.98277900
C	-2.45388000	0.49530500	-2.20057500
O	-2.13135500	-0.60326900	-1.64460500
O	-1.82164100	1.57649400	-2.03136600
C	-8.23142800	-1.55454900	1.18249800
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O	-9.40276300	-1.83388400	1.80279800
H	-9.19949900	-1.90913100	2.75042400
O	1.51467500	0.01717900	-2.09157700
H	2.34278400	0.50619900	-2.16440300
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C	-2.63717500	0.78365900	2.24765500
O	-1.81624800	0.96565400	1.33687100
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H	-2.70507700	1.49515500	3.08602900
C	-4.38025800	-0.36117200	3.50315100
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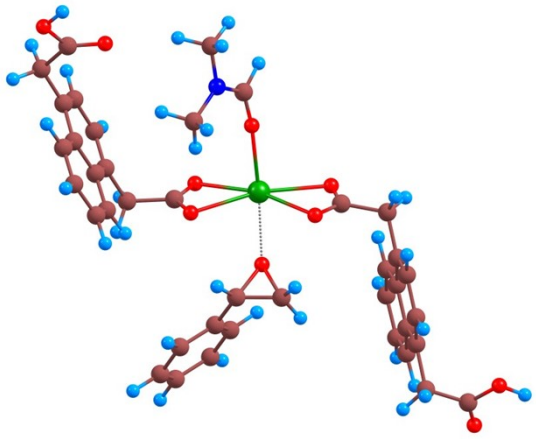
EM-2



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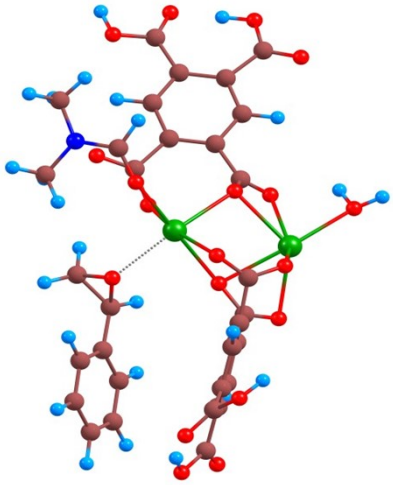
EM-3



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O	1.69570000	1.09678600	-0.82319400
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O	-6.82704600	-1.12825600	3.29537000
O	2.41511800	-2.64268500	-0.88492900
O	1.65470000	-5.03080000	0.22519900
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C	2.86203900	1.56495900	-0.59168800
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H	-4.32157200	-0.95882200	2.96423100
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O	8.82537000	0.47675900	-1.11229800
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C	6.31497700	-1.15133300	-0.45600700
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O	-6.82136000	-1.37359500	-2.23199400
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C	-6.83944700	-0.84829200	-1.13754800
C	-5.65149500	-1.03645400	-0.19380700
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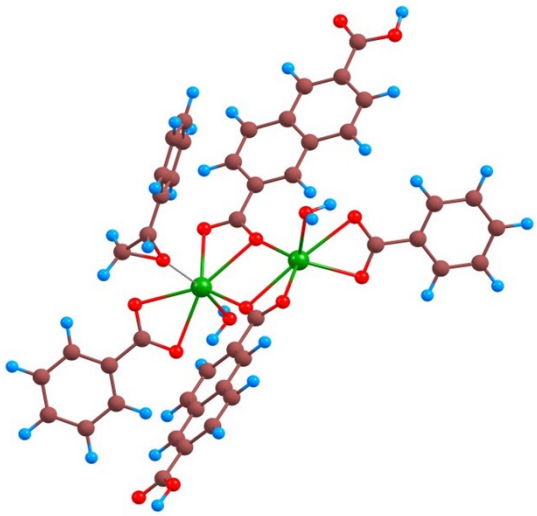
EM-4



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O	-1.25438100	-2.73327000	-0.65555600
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References:

1 G. M. Sheldrick, *Acta Crystallogr., Sect. A: Found. Adv*., 2015, 71, 3-8.

2 A. L. Spek, *J. Appl. Crystallogr.*, 2003, **36**, 7.

3 M. G. Sheldrick, A Short History of SHELX. *Acta Cryst.,* 2008, **A64**, 112-122.

4 O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard and H. Puschmann, *J. Appl. Crystallogr.*, 2009, **42**, 339342.

5 J. L. Farrugia, *J. Appl. Crystallogr*. 2012, **45**, 849-854.

6 A. V. Blatov, Nanocluster Analysis of Intermetallic Structures with the Program Package TOPOS. *Struct. Chem.* 2012, **23**, 955-963.

7 R. Bader*, J. Phys. Chem. A*, 1998, **102**, 7314-7323.

8 P. S. V. Kumar, V. Raghavendra and V. Subhramanian, *Journal of Chemical Sciences*, 2016, **128**, 1527-1536.

9 A. Banerjee, T. Ash, T. Debnath and A. K. Das, *Int. J. Hydrog. Energy*. 2021, **46**, 17827-17839.