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

Enhancing the electrocatalytic OER activity of Co-MOFs through labile solvents coordination

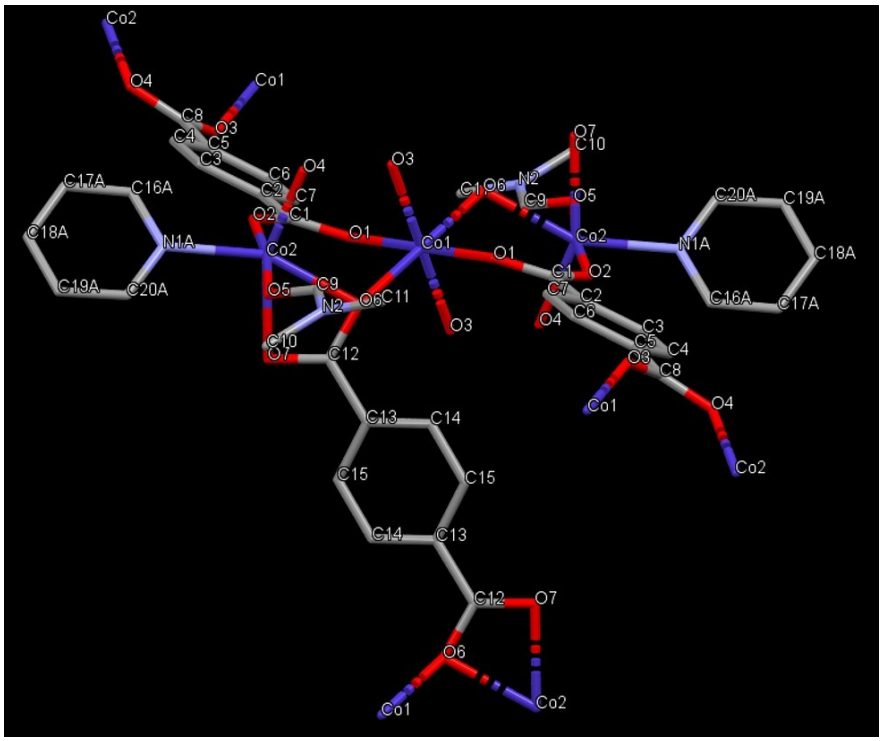

Figure S1. Molecular structure in the crystal lattice of **Co-MOF-1**. C (grey), H (white), N (blue), O (red) and Co (dark blue). Hydrogen atoms are removed for clarity.

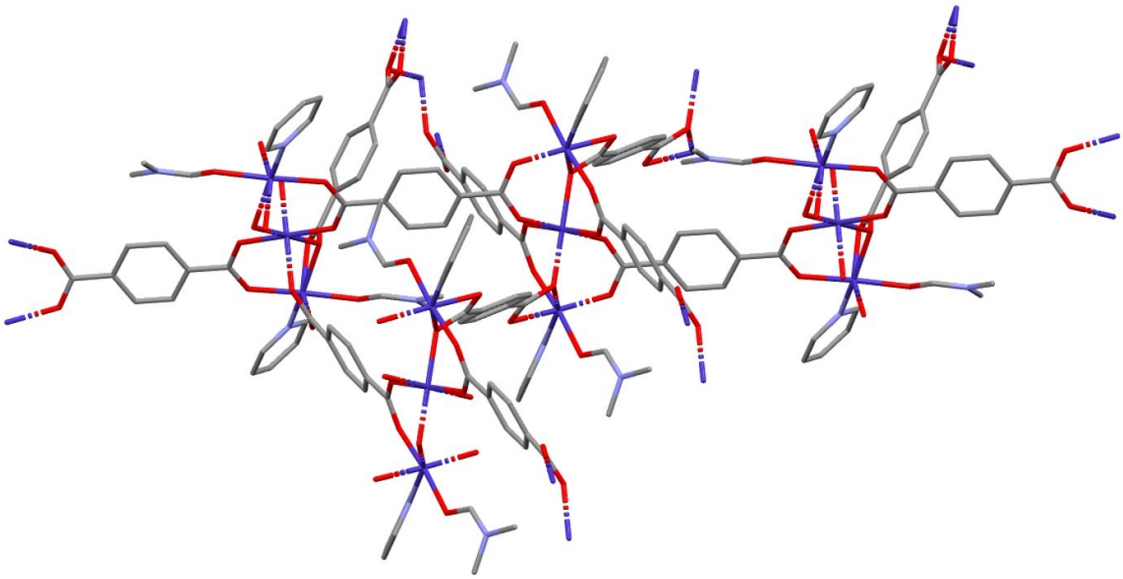

Figure S2. The coordination of BDC, pyridine and DMF with different cobalt centre of **Co-MOF-1**. C (grey), H (white), N (blue), O (red) and Co (dark blue). Hydrogen atoms are removed for clarity.

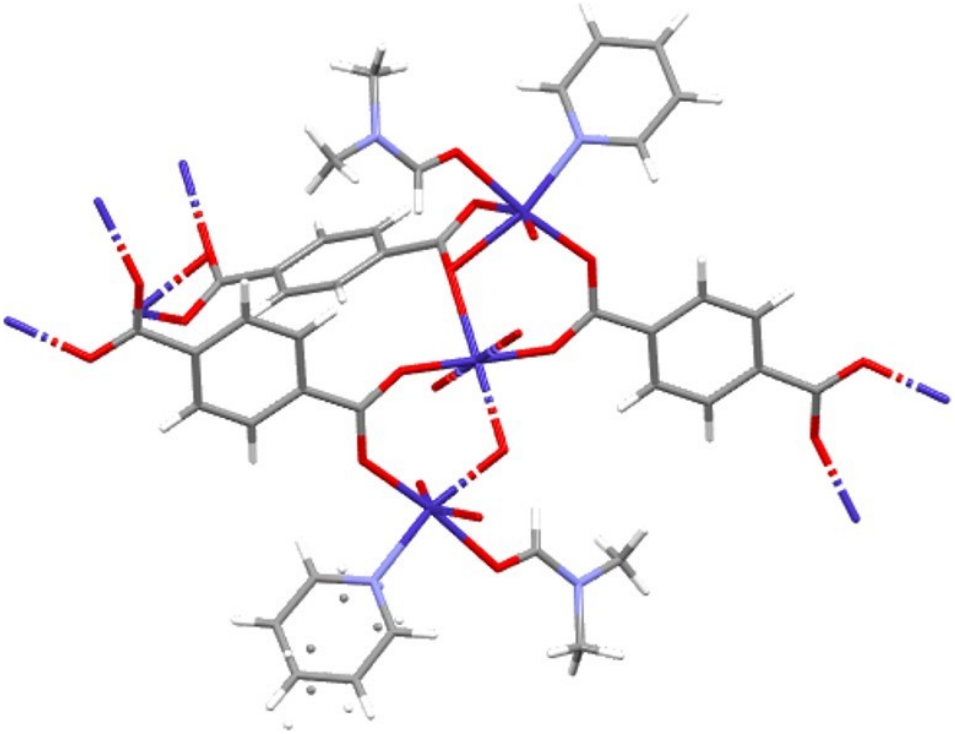

Figure S3. Molecular structure of **Co-MOF-1** in the crystal lattice. C (grey), H (white), N (blue), O (red) and Co (dark blue).

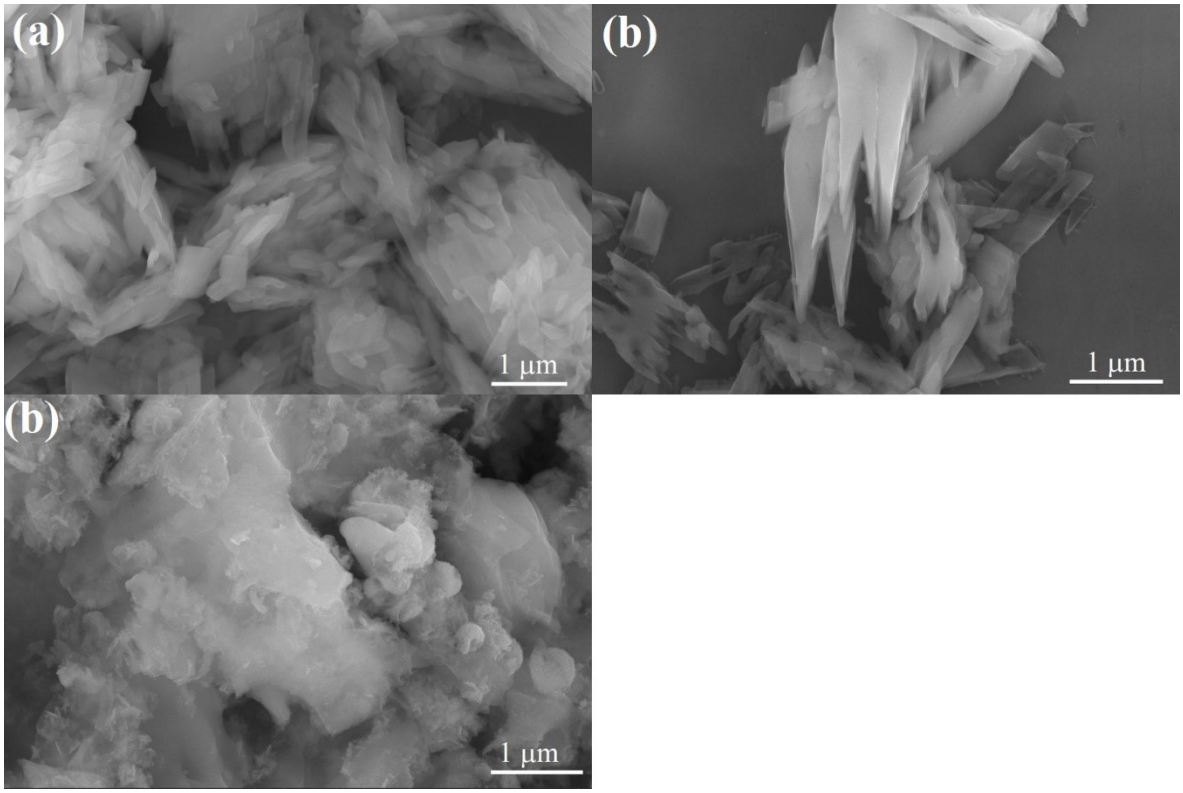

Figure S4. FE-SEM images of (a) **Co-MOF-1,** (b) **Co-MOF-2** and (c) Co-MOF-1 (after catalysis)

Table S1. Crystal data and structure refinement for **Co-MOF-1** (CCDC No 2246026).

Identification code	**Co-MOF-1**	
Empirical formula	$C_{40}H_{36}Co_3N_4O_{14}$	
Formula weight	973.52	
Temperature	220(2) K	
Wavelength	0.610 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 14.496(3) Å	α= 90°.
	b = 9.7410(19) Å	β= 109.61(3)°.
	c = 16.453(3) Å	γ = 90°.
Volume	2188.4(8) $Å^3$	
Z	2	
Density (calculated)	1.477 Mg/m^3	
Absorption coefficient	0.782 mm^{-1}	
F(000)	994	
Crystal size	0.105 x 0.065 x 0.020 mm^3	
Theta range for data collection	1.393 to 24.999°.	
Index ranges	-20<=h<=20, -13<=k<=13, -22<=l<=22	
Reflections collected	21779	
Independent reflections	6077 [R(int) = 0.0908]	
Completeness to theta = 21.469°	99.3 %	
Absorption correction	Empirical	
Max. and min. transmission	1.000 and 0.862	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6077 / 178 / 334	
Goodness-of-fit on F^2	1.001	
Final R indices [I>2sigma(I)]	R1 = 0.0662, wR2 = 0.1859	
R indices (all data)	R1 = 0.0779, wR2 = 0.1934	
Extinction coefficient	n/a	
Largest diff. peak and hole	2.616 and -0.716 e.$Å^{-3}$	

Table S2. Crystal data and structure refinement for **Co-MOF-2**.

Identification code	**Co-MOF-2**	
Empirical formula	C38 H36 Co3 N2 O16	
Formula weight	953.48	
Temperature	220(2) K	
Wavelength	0.630 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 33.257(7) Å	α= 90°.
	b = 9.810(2) Å	β= 97.78(3)°.
	c = 17.964(4) Å	γ = 90°.
Volume	5807(2) $Å^3$	
Z	4	
Density (calculated)	1.091 Mg/m^3	
Absorption coefficient	0.643 mm^{-1}	
F(000)	1948	
Crystal size	0.125 x 0.058 x 0.015 mm^3	
Theta range for data collection	1.096 to 26.495°.	
Index ranges	-46<=h<=46, -12<=k<=12, -25<=l<=25	
Reflections collected	24935	
Independent reflections	7446 [R(int) = 0.1283]	
Completeness to theta = 22.210°	98.9 %	
Absorption correction	Empirical	
Max. and min. transmission	1.000 and 0.799	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7446 / 0 / 271	
Goodness-of-fit on F^2	0.828	
Final R indices [I>2sigma(I)]	R1 = 0.0816, wR2 = 0.2140	
R indices (all data)	R1 = 0.1967, wR2 = 0.2381	
Extinction coefficient	n/a	
Largest diff. peak and hole	1.166 and -0.861 $e.Å^{-3}$	

S. No	Catalyst	Org. linker	Substrate	Over potential η at 10mA	Tafel mV/dec	Reference
1	Ultrathin 2D Co-MOF	Terephthalate	GCE	371	74	1
2	CoBDC	Terephthalate	GCE	334	-	2
3	CoMONs	Terephthalate	Carbon paper	309	75.71	3
4	CoBDC-Fc-NF	Terephthalate and Ferrocene carboxylic acid	Nickel Foam	178	51	4
5	Ti_3C_2Tx−CoBDC	Citrate	GCE	410	48.2	5
6	Co-BPDC/Co BDC-3	1,4-benzenedicarboxylic acid and 4,4′-biphenyldicarboxylate	GCE	335	72.1	6
7	UTSA-16	Citrate	GCE	408	77	7
8	Co-MOF NF	Terephthalic acid	Nickel foam	311 @50mA	77	8
9	MAF-X27-OH	1H,5H-benzo(1,2 d:4,5-d′)bistriazole	GCE	387	60	9
10	Co-OBA/C	4,4'-oxybis(benzoic acid), and imidazole	GCE	774 (vs Ag/AgCl)	85.7 (vs Ag/AgCl)	10
11	Co-MOF@CNTs (5 wt%)	benzimidazole	GCE	340	69	11
12	CoTPA-D	Terephthalate	Carbon cloth	273	67	12
13	Co-MOF-1	Terephthalate	GCE	294	57.5	**This work**

Table S3. Comparison of Co-MOFs electrocatalytic OER activity.

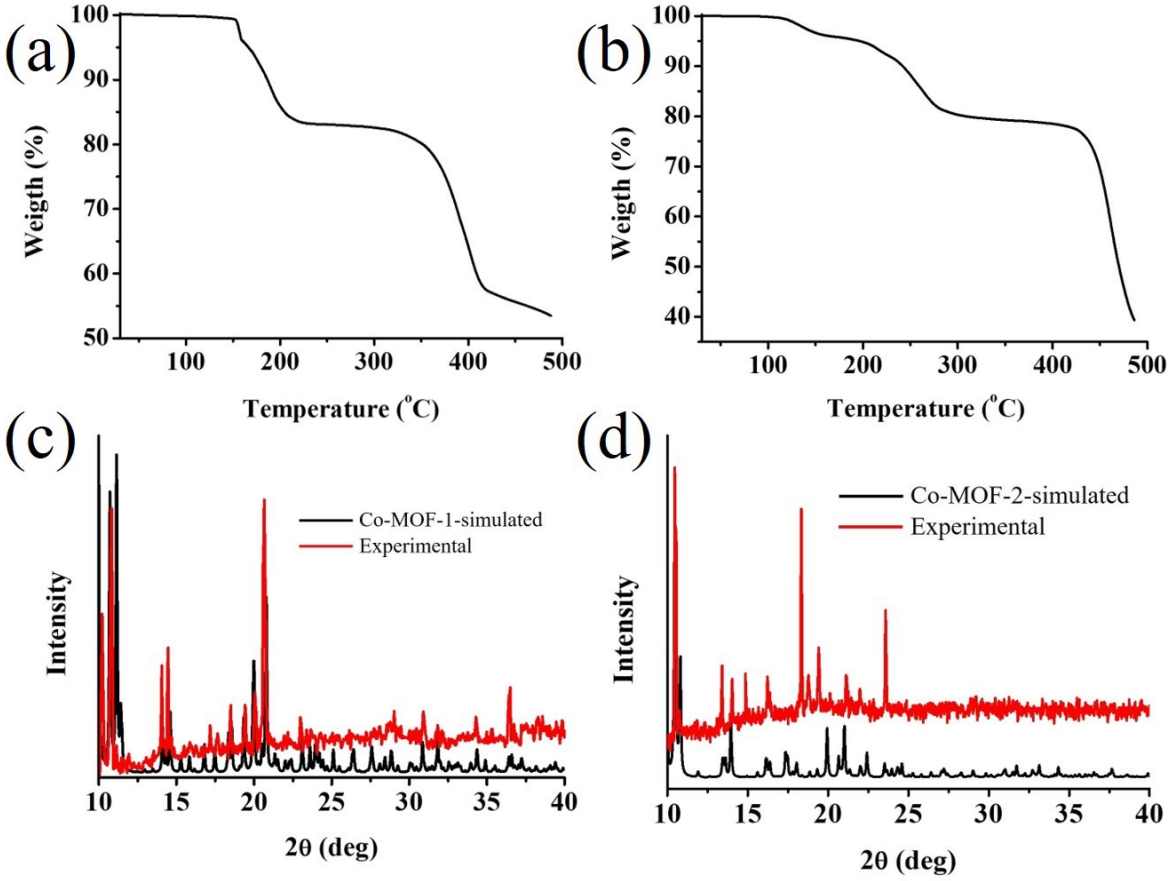

Figure S5. (a, b) PXRD and (c, d) TGA of (a, c) **Co-MOF-1** and (b, d) **Co-MOF-2**.

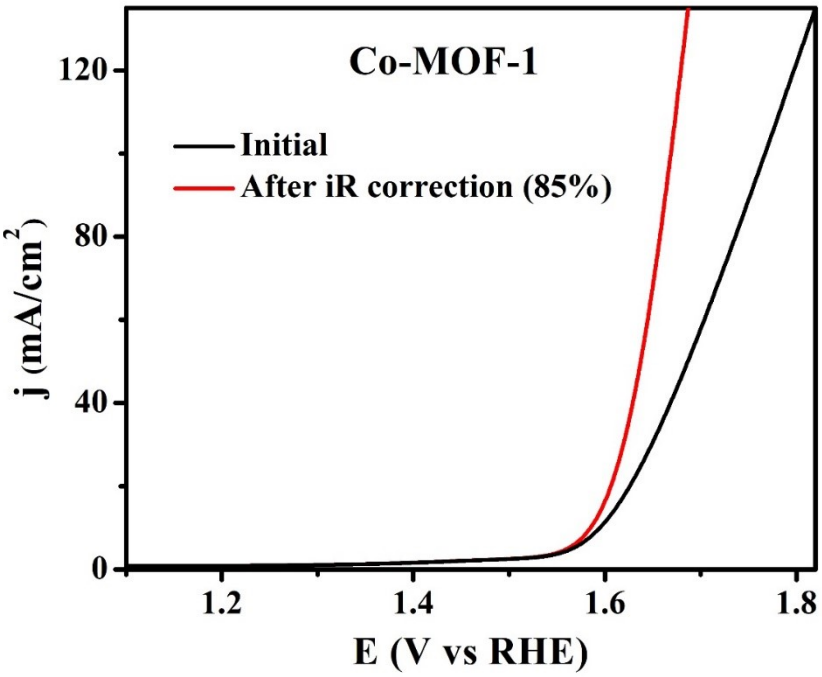

Figure S6. OER polarization curves of **Co-MOF-1** before and after iR correction.

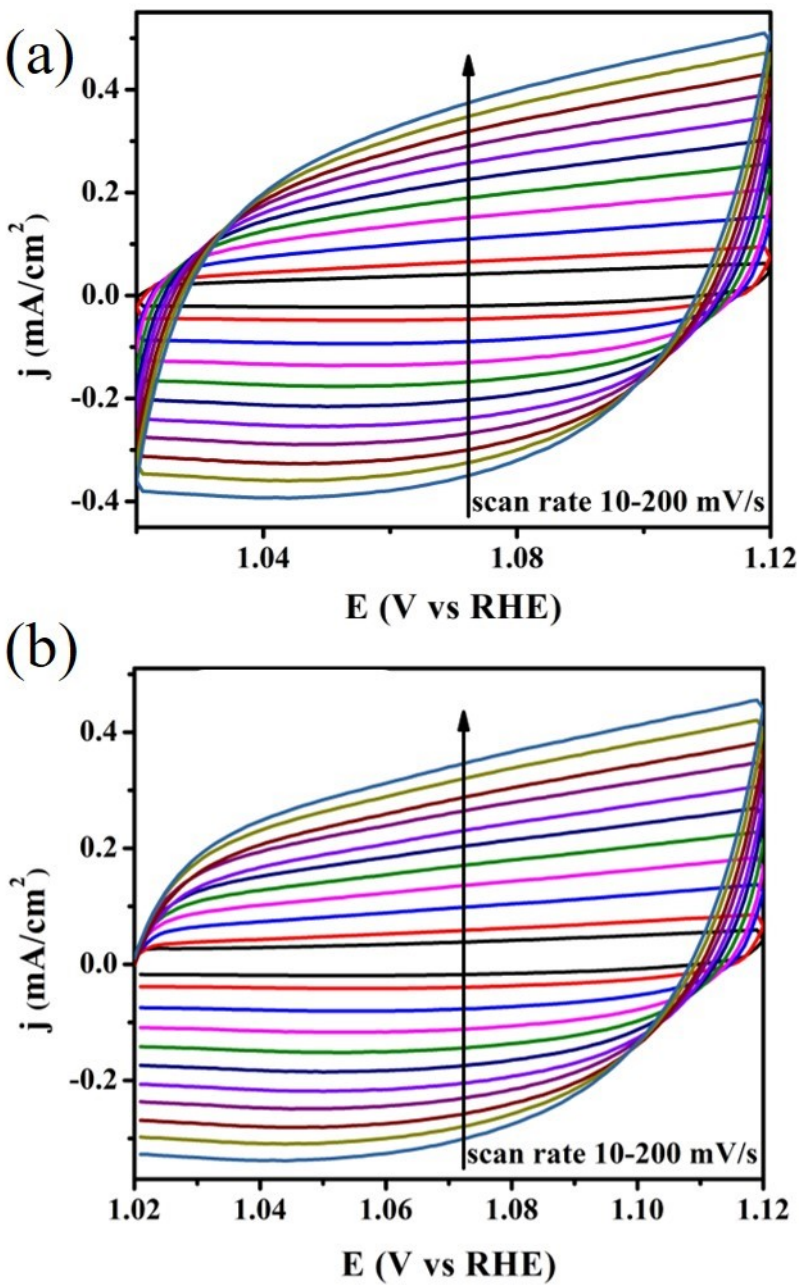

Figure S7. Double layer capacitance and capacitive currents as a functional of scan rate.

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