

Supporting Information for:

Synthesis of Cobalt Complex Containing trans-cinnamate and Its Electrocatalytic Activity for Oxygen Evolution Reaction

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Table S1. Crystal data and structure refinement for **1**.

Empirical formula	$\text{C}_{44} \text{H}_{39} \text{Co}_2 \text{N}_6 \text{O}_{11.5}$	
Formula weight	953.67	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	$a = 9.46580(10)$ Å	$\alpha = 108.1025(10)^\circ$.
	$b = 14.3195(2)$ Å	$\beta = 101.8118(9)^\circ$.
	$c = 18.1311(3)$ Å	$\gamma = 100.4024(10)^\circ$.
Volume	$2206.34(6)$ Å ³	
Z	2	
Density (calculated)	1.436 Mg/m ³	
Absorption coefficient	0.820 mm ⁻¹	
F(000)	982	
Crystal size	0.310 x 0.260 x 0.230 mm ³	
Theta range for data collection	1.230 to 28.369°.	
Index ranges	$-12 \leq h \leq 12$, $-18 \leq k \leq 19$, $-24 \leq l \leq 24$	
Reflections collected	30393	
Independent reflections	10919 [R(int) = 0.0978]	
Completeness to theta = 25.242°	99.8 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	10919 / 0 / 590	
Goodness-of-fit on F ²	0.886	
Final R indices [I>2sigma(I)]	R1 = 0.0551, wR2 = 0.1164	
R indices (all data)	R1 = 0.1225, wR2 = 0.1376	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.886 and -0.746 e.Å ⁻³	

Table S2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **1**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Co(1)	-1483(1)	-152(1)	3557(1)	32(1)
Co(2)	2337(1)	1062(1)	3877(1)	31(1)
N(1)	-4052(3)	931(3)	4333(2)	51(1)
N(2)	-3926(3)	-240(2)	3170(2)	34(1)
N(3)	3729(3)	68(2)	3344(2)	33(1)
C(1)	-4759(3)	240(3)	3608(2)	32(1)
C(2)	-4682(4)	-936(3)	2440(2)	48(1)
C(3)	-6193(4)	-1182(3)	2153(2)	58(1)
C(4)	3047(4)	-663(3)	2625(2)	45(1)
N(4)	4155(4)	3602(3)	4946(2)	72(1)
N(5)	4936(4)	4103(3)	3998(2)	67(1)
N(6)	3760(3)	2350(2)	3706(2)	44(1)
C(5)	4274(4)	3338(3)	4203(3)	50(1)
C(6)	5078(6)	3838(5)	3258(4)	91(2)
C(7)	4624(6)	2861(5)	2715(3)	83(2)
C(8)	3955(5)	2138(4)	2971(3)	59(1)
O(1)	-976(2)	1163(2)	4523(2)	42(1)
O(2)	1177(3)	2050(2)	4460(2)	40(1)
C(9)	62(4)	1970(3)	4733(2)	36(1)
C(10)	-137(4)	2873(3)	5330(2)	43(1)
C(11)	535(4)	3814(3)	5481(2)	45(1)
C(12)	213(5)	4733(3)	5994(2)	48(1)
C(13)	1040(5)	5694(3)	6103(3)	61(1)
C(14)	706(7)	6563(4)	6561(3)	74(2)
C(15)	-448(8)	6458(5)	6906(3)	89(2)
C(16)	-1254(7)	5521(4)	6817(3)	90(2)
C(17)	-934(6)	4669(4)	6366(3)	71(1)
O(3)	3671(2)	1438(2)	5045(1)	34(1)
O(4)	-2035(2)	-858(2)	4374(1)	35(1)
C(18)	3191(3)	1481(3)	5655(2)	29(1)

C(19)	4014(4)	2315(3)	6426(2)	39(1)
C(20)	5444(4)	2768(3)	6647(2)	44(1)
C(21)	6283(4)	3591(3)	7415(2)	43(1)
C(22)	7757(4)	3654(4)	7793(3)	62(1)
C(23)	8520(5)	4425(4)	8516(3)	81(2)
C(24)	7856(6)	5149(4)	8871(3)	89(2)
C(25)	6395(5)	5103(4)	8512(3)	77(2)
C(26)	5613(4)	4322(3)	7793(2)	53(1)
O(5)	-1755(3)	-1488(2)	2629(1)	40(1)
O(6)	160(3)	-2073(2)	3074(2)	51(1)
C(27)	-1077(4)	-2176(3)	2609(2)	39(1)
C(28)	-1889(4)	-3190(3)	1962(2)	45(1)
C(29)	-1725(4)	-4062(3)	1999(2)	47(1)
C(30)	-2543(4)	-5073(3)	1399(2)	47(1)
C(31)	-2646(5)	-5902(3)	1635(3)	65(1)
C(32)	-3423(7)	-6855(4)	1105(4)	87(2)
C(33)	-4101(6)	-7013(4)	317(4)	94(2)
C(34)	-3983(6)	-6207(4)	51(3)	80(2)
C(35)	-3212(5)	-5243(3)	597(3)	60(1)
O(7)	1087(3)	695(2)	2709(1)	42(1)
O(8)	-1254(3)	605(2)	2775(2)	50(1)
C(36)	-231(4)	732(3)	2454(2)	38(1)
C(37)	-582(6)	1000(5)	1728(3)	89(2)
C(38)	515(7)	1219(5)	1341(3)	94(2)
C(39)	491(8)	1655(5)	678(3)	97(2)
C(40)	-573(10)	2100(6)	466(4)	143(3)
C(41)	-670(9)	2416(5)	-168(4)	118(3)
C(42)	258(8)	2179(6)	-651(3)	106(3)
C(43)	1344(10)	1782(7)	-466(5)	141(3)
C(44)	1589(8)	1574(6)	264(5)	131(3)
OW1	859(2)	-174(2)	3999(1)	30(1)
OW2	-4540(20)	8(7)	419(9)	219(9)
OW3	-6230(40)	610(40)	570(20)	390(30)
OW4	-6295(18)	-60(13)	873(10)	81(9)
OW5	-2702(15)	292(11)	-48(8)	45(6)

OW6	-2459(14)	491(10)	1404(7)	88(6)
OW7	-3430(20)	288(13)	546(9)	64(7)
OW8	-4722(19)	220(16)	1030(19)	120(11)

Table S3. Bond lengths [Å] and angles [°] for **1**.

Co(1)-O(1)	2.032(2)
Co(1)-O(5)	2.048(2)
Co(1)-O(8)	2.056(3)
Co(1)-O(4)	2.133(2)
Co(1)-OW1	2.207(2)
Co(1)-N(2)	2.244(3)
Co(2)-O(7)	2.053(2)
Co(2)-O(3)	2.078(2)
Co(2)-O(2)	2.105(2)
Co(2)-OW1	2.148(2)
Co(2)-N(6)	2.223(3)
Co(2)-N(3)	2.244(3)
N(1)-C(1)	1.321(4)
N(2)-C(2)	1.338(4)
N(2)-C(1)	1.356(4)
N(3)-C(4)	1.333(4)
N(3)-C(1)#1	1.363(4)
C(2)-C(3)	1.357(5)
C(3)-C(4)#2	1.361(5)
N(4)-C(5)	1.317(5)
N(5)-C(6)	1.319(6)
N(5)-C(5)	1.353(5)
N(6)-C(8)	1.331(5)
N(6)-C(5)	1.353(5)
C(6)-C(7)	1.365(7)
C(7)-C(8)	1.367(6)
O(1)-C(9)	1.270(4)
O(2)-C(9)	1.255(4)
C(9)-C(10)	1.477(5)
C(10)-C(11)	1.298(5)
C(11)-C(12)	1.480(5)
C(12)-C(13)	1.387(6)
C(12)-C(17)	1.394(6)

C(13)-C(14)	1.395(6)
C(14)-C(15)	1.374(7)
C(15)-C(16)	1.361(7)
C(16)-C(17)	1.364(6)
O(3)-C(18)	1.269(4)
O(4)-C(18)#3	1.261(4)
C(18)-C(19)	1.472(5)
C(19)-C(20)	1.308(5)
C(20)-C(21)	1.466(5)
C(21)-C(26)	1.393(5)
C(21)-C(22)	1.396(5)
C(22)-C(23)	1.372(6)
C(23)-C(24)	1.368(7)
C(24)-C(25)	1.382(7)
C(25)-C(26)	1.378(5)
O(5)-C(27)	1.265(4)
O(6)-C(27)	1.249(4)
C(27)-C(28)	1.498(5)
C(28)-C(29)	1.306(5)
C(29)-C(30)	1.467(5)
C(30)-C(31)	1.376(6)
C(30)-C(35)	1.385(6)
C(31)-C(32)	1.364(7)
C(32)-C(33)	1.370(7)
C(33)-C(34)	1.378(7)
C(34)-C(35)	1.381(6)
O(7)-C(36)	1.255(4)
O(8)-C(36)	1.242(4)
C(36)-C(37)	1.474(6)
C(37)-C(38)	1.409(7)
C(37)-OW6	1.695(13)
C(38)-C(39)	1.515(8)
C(39)-C(40)	1.339(8)
C(39)-C(44)	1.402(8)
C(40)-C(41)	1.352(8)

C(41)-C(42)	1.376(9)
C(42)-C(43)	1.297(10)
C(43)-C(44)	1.428(9)
O(1)-Co(1)-O(5)	173.61(10)
O(1)-Co(1)-O(8)	92.80(11)
O(5)-Co(1)-O(8)	88.59(11)
O(1)-Co(1)-O(4)	84.25(10)
O(5)-Co(1)-O(4)	95.29(9)
O(8)-Co(1)-O(4)	170.88(10)
O(1)-Co(1)-OW1	85.75(9)
O(5)-Co(1)-OW1	87.87(9)
O(8)-Co(1)-OW1	100.16(9)
O(4)-Co(1)-OW1	88.25(8)
O(1)-Co(1)-N(2)	95.03(10)
O(5)-Co(1)-N(2)	91.30(10)
O(8)-Co(1)-N(2)	85.56(10)
O(4)-Co(1)-N(2)	86.10(9)
OW1-Co(1)-N(2)	174.19(9)
O(7)-Co(2)-O(3)	177.96(9)
O(7)-Co(2)-O(2)	97.99(10)
O(3)-Co(2)-O(2)	83.51(9)
O(7)-Co(2)-OW1	90.99(9)
O(3)-Co(2)-OW1	90.43(8)
O(2)-Co(2)-OW1	88.60(9)
O(7)-Co(2)-N(6)	86.41(11)
O(3)-Co(2)-N(6)	92.22(10)
O(2)-Co(2)-N(6)	90.08(11)
OW1-Co(2)-N(6)	176.90(10)
O(7)-Co(2)-N(3)	86.31(10)
O(3)-Co(2)-N(3)	92.16(9)
O(2)-Co(2)-N(3)	175.42(10)
OW1-Co(2)-N(3)	92.93(9)
N(6)-Co(2)-N(3)	88.59(11)
C(2)-N(2)-C(1)	116.0(3)

C(2)-N(2)-Co(1)	115.2(2)
C(1)-N(2)-Co(1)	128.5(2)
C(4)-N(3)-C(1)#1	116.4(3)
C(4)-N(3)-Co(2)	116.1(2)
C(1)#1-N(3)-Co(2)	126.5(2)
N(1)-C(1)-N(2)	117.7(3)
N(1)-C(1)-N(3)#2	118.1(3)
N(2)-C(1)-N(3)#2	124.2(3)
N(2)-C(2)-C(3)	123.1(4)
C(2)-C(3)-C(4)#2	117.6(4)
N(3)-C(4)-C(3)#1	122.6(3)
C(6)-N(5)-C(5)	115.9(4)
C(8)-N(6)-C(5)	116.0(3)
C(8)-N(6)-Co(2)	114.6(3)
C(5)-N(6)-Co(2)	128.7(3)
N(4)-C(5)-N(6)	119.6(3)
N(4)-C(5)-N(5)	115.7(4)
N(6)-C(5)-N(5)	124.7(4)
N(5)-C(6)-C(7)	124.0(4)
C(6)-C(7)-C(8)	116.2(5)
N(6)-C(8)-C(7)	123.2(5)
C(9)-O(1)-Co(1)	129.4(2)
C(9)-O(2)-Co(2)	136.8(2)
O(2)-C(9)-O(1)	125.4(3)
O(2)-C(9)-C(10)	119.9(3)
O(1)-C(9)-C(10)	114.8(3)
C(11)-C(10)-C(9)	125.8(4)
C(10)-C(11)-C(12)	126.8(4)
C(13)-C(12)-C(17)	117.9(4)
C(13)-C(12)-C(11)	120.1(4)
C(17)-C(12)-C(11)	121.9(4)
C(12)-C(13)-C(14)	120.5(5)
C(15)-C(14)-C(13)	119.3(5)
C(16)-C(15)-C(14)	121.0(5)
C(15)-C(16)-C(17)	119.8(6)

C(16)-C(17)-C(12)	121.5(5)
C(18)-O(3)-Co(2)	125.21(19)
C(18)#3-O(4)-Co(1)	132.9(2)
O(4)#3-C(18)-O(3)	123.1(3)
O(4)#3-C(18)-C(19)	119.1(3)
O(3)-C(18)-C(19)	117.8(3)
C(20)-C(19)-C(18)	125.7(3)
C(19)-C(20)-C(21)	126.4(4)
C(26)-C(21)-C(22)	118.3(4)
C(26)-C(21)-C(20)	120.4(3)
C(22)-C(21)-C(20)	121.2(4)
C(23)-C(22)-C(21)	120.4(4)
C(24)-C(23)-C(22)	120.6(5)
C(23)-C(24)-C(25)	120.3(4)
C(26)-C(25)-C(24)	119.5(5)
C(25)-C(26)-C(21)	120.9(4)
C(27)-O(5)-Co(1)	129.2(2)
O(6)-C(27)-O(5)	125.8(3)
O(6)-C(27)-C(28)	119.7(4)
O(5)-C(27)-C(28)	114.5(3)
C(29)-C(28)-C(27)	124.4(4)
C(28)-C(29)-C(30)	126.2(4)
C(31)-C(30)-C(35)	117.8(4)
C(31)-C(30)-C(29)	118.8(4)
C(35)-C(30)-C(29)	123.4(4)
C(32)-C(31)-C(30)	121.2(5)
C(31)-C(32)-C(33)	120.6(5)
C(32)-C(33)-C(34)	119.9(5)
C(33)-C(34)-C(35)	118.9(5)
C(34)-C(35)-C(30)	121.6(5)
C(36)-O(7)-Co(2)	129.2(2)
C(36)-O(8)-Co(1)	129.3(2)
O(8)-C(36)-O(7)	126.1(3)
O(8)-C(36)-C(37)	116.7(4)
O(7)-C(36)-C(37)	117.1(4)

C(38)-C(37)-C(36)	121.7(4)
C(38)-C(37)-OW6	133.9(6)
C(36)-C(37)-OW6	99.5(6)
C(37)-C(38)-C(39)	131.1(5)
C(40)-C(39)-C(44)	119.0(6)
C(40)-C(39)-C(38)	121.6(6)
C(44)-C(39)-C(38)	119.4(6)
C(39)-C(40)-C(41)	121.8(7)
C(40)-C(41)-C(42)	118.5(7)
C(43)-C(42)-C(41)	122.5(7)
C(42)-C(43)-C(44)	119.1(8)
C(39)-C(44)-C(43)	117.5(7)
Co(2)-OW1-Co(1)	109.64(10)

Symmetry transformations used to generate equivalent atoms:

#1 $x+1, y, z$ #2 $x-1, y, z$ #3 $-x, -y, -z+1$ #4 $-x-1, -y, -z$

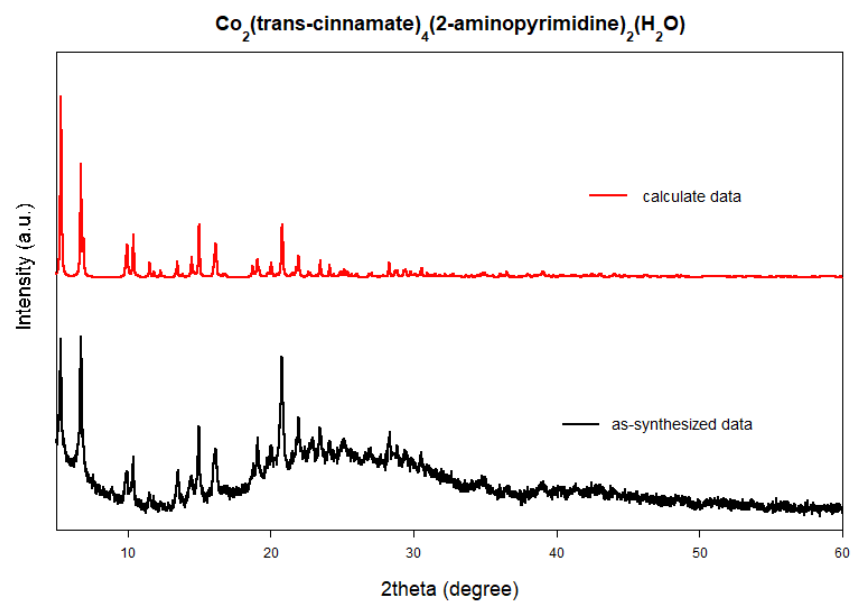


Figure S1: The powder XRD pattern of **1**.

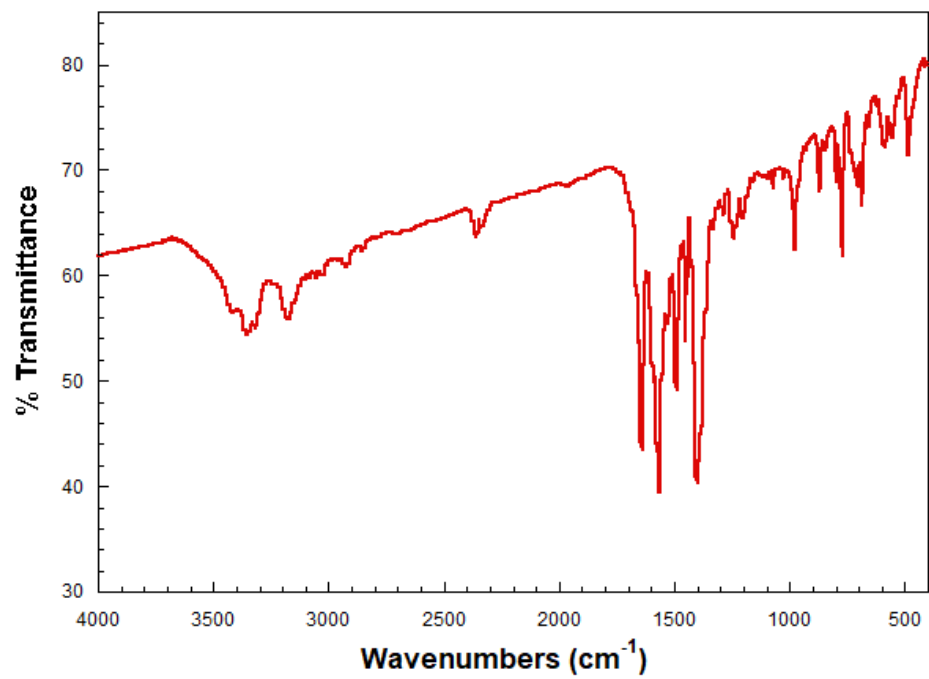


Figure S2: IR of **1**.