Supporting Information for

Molecular Coordination Inheritance of Single Co Atom Catalysts for Two-Electron Oxygen Reduction Reaction

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Fig. S1–S9

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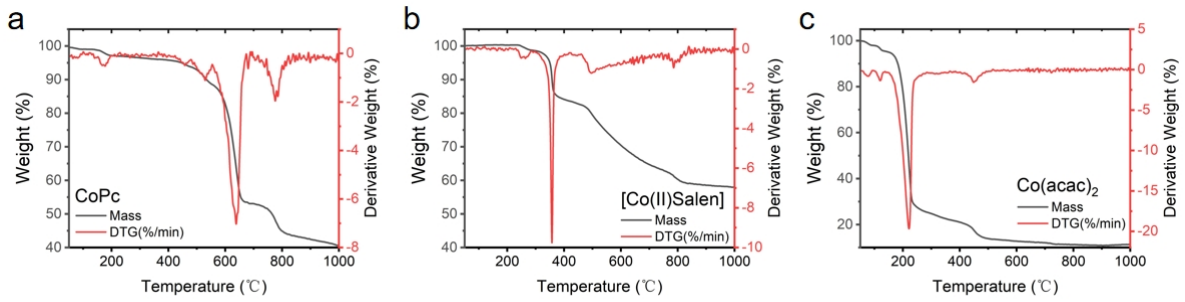

Fig. S1. TG and DTG curves of (a) CoPc, (b) [Co(II)Salen] and (c) $Co(acac)_2$ with the heating rate of 10 °C/min in N_2 atmosphere.

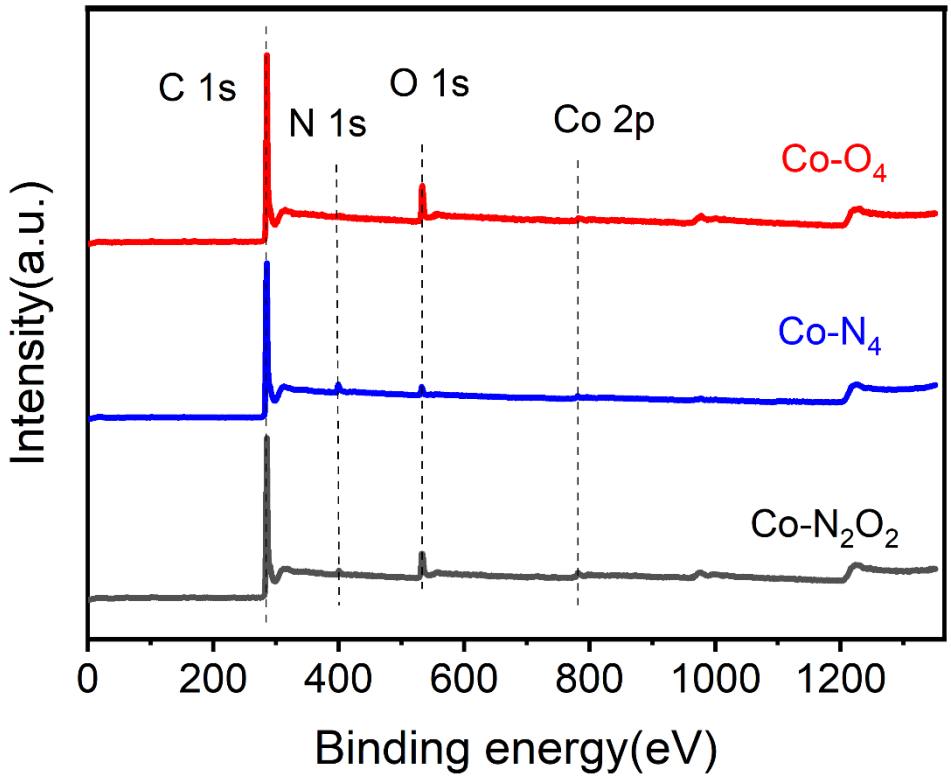

Fig. S2. XPS survey spectra of Co-N_2O_2, Co-N_4 and Co-O_4 catalysts.

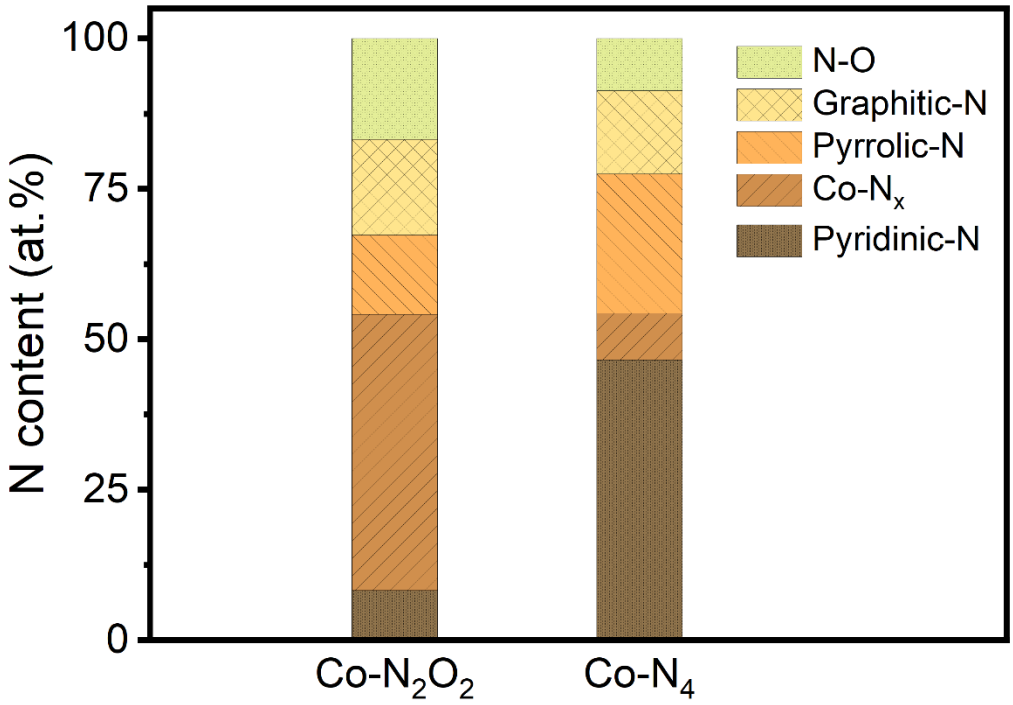

Fig. S3. The proportion of different N species of Co-N_2O_2 and Co-N_4 catalysts.

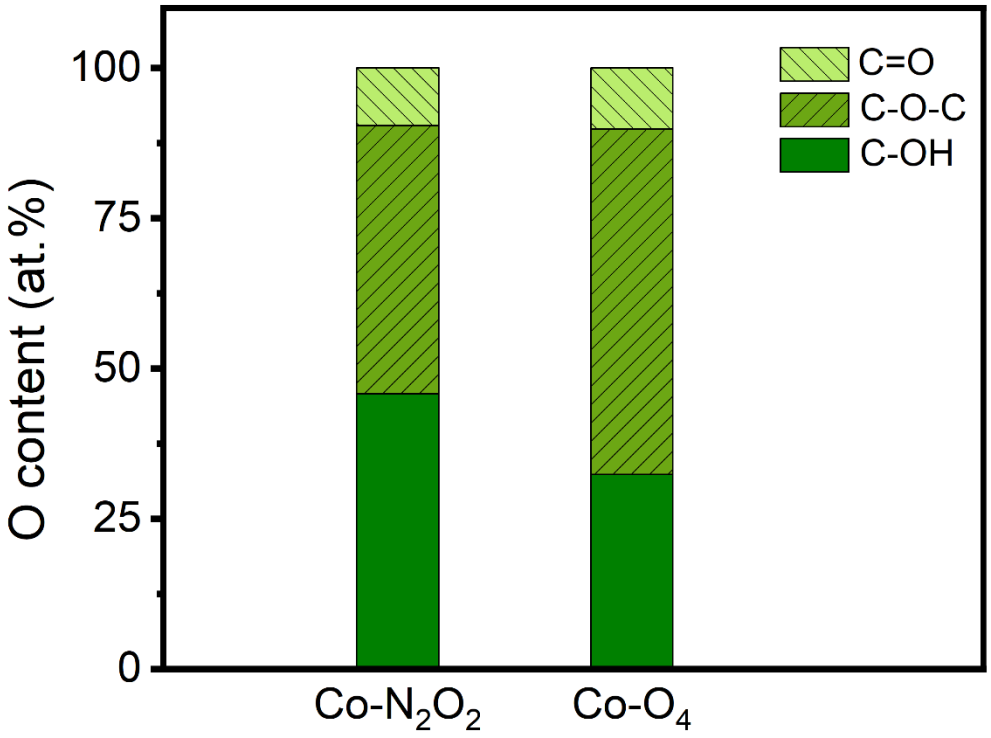

Fig. S4. The proportion of different O species of Co-N_2O_2 and Co-O_4 catalysts.

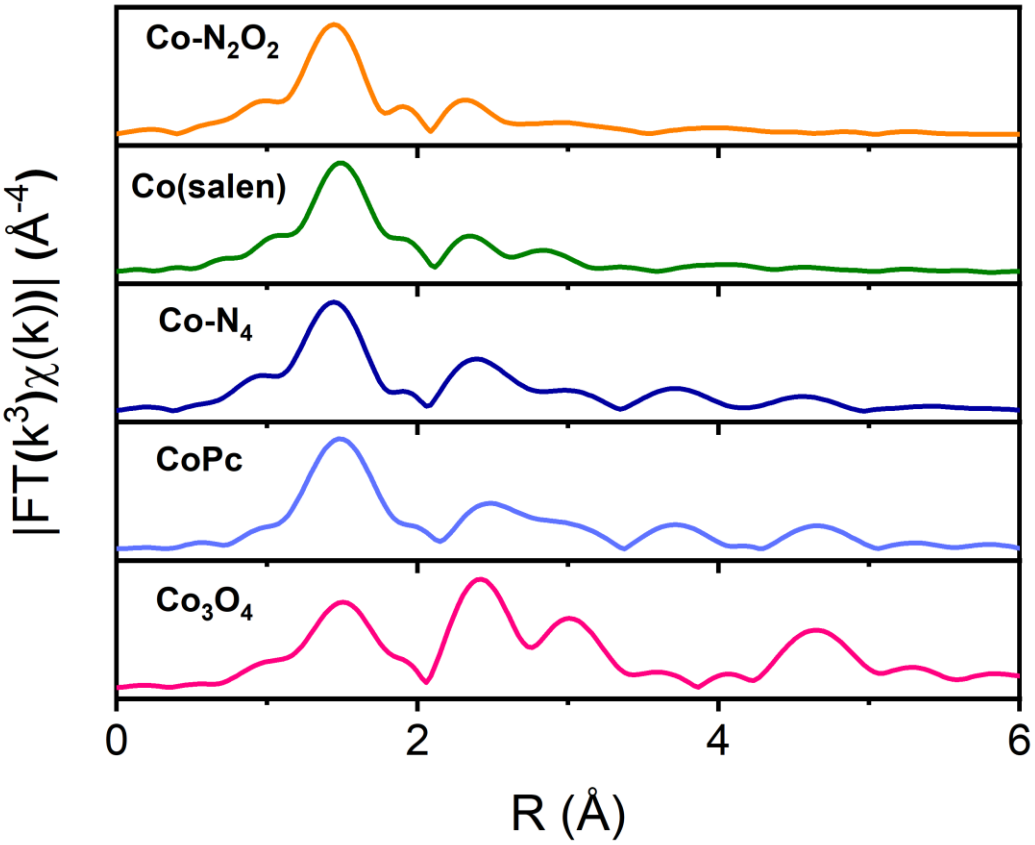

Fig. S5. FT k^2-weighted and fitting extended XAFS (EXAFS) spectra of the Co-N_2O_2, Co-N_4 catalysts, and [Co(II)Salen], CoPc, Co_3O_4 reference.

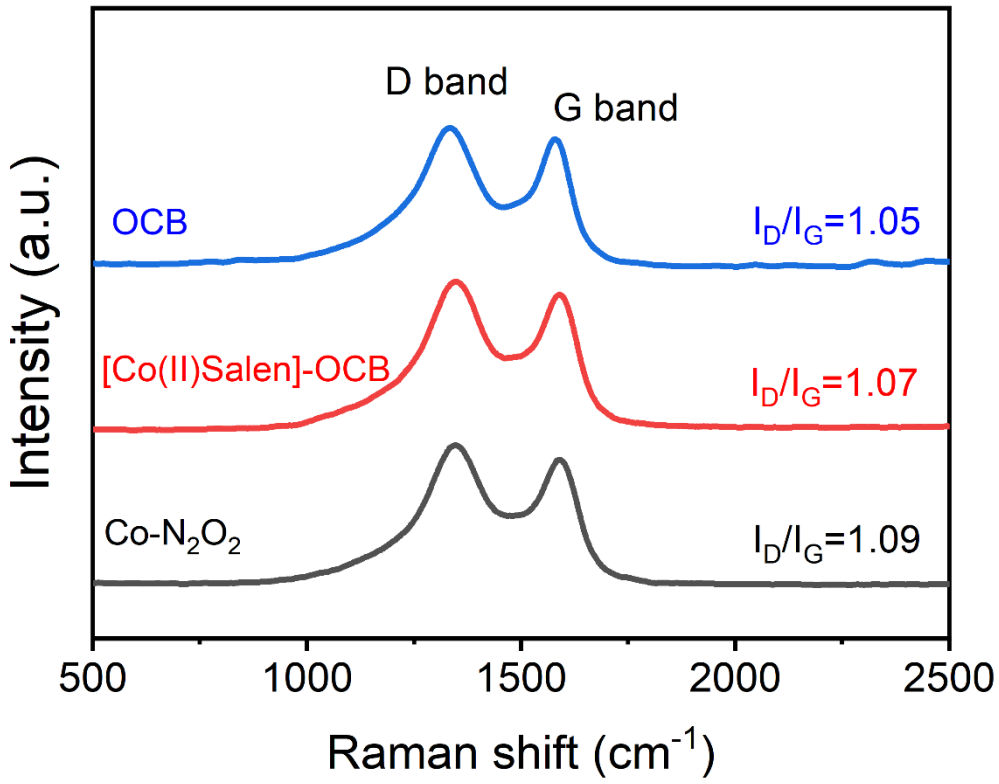

Fig. S6. Raman spectra of the OCB substrate, [Co(II)Salen]-OCB precursor, and Co-N_2O_2 catalyst.

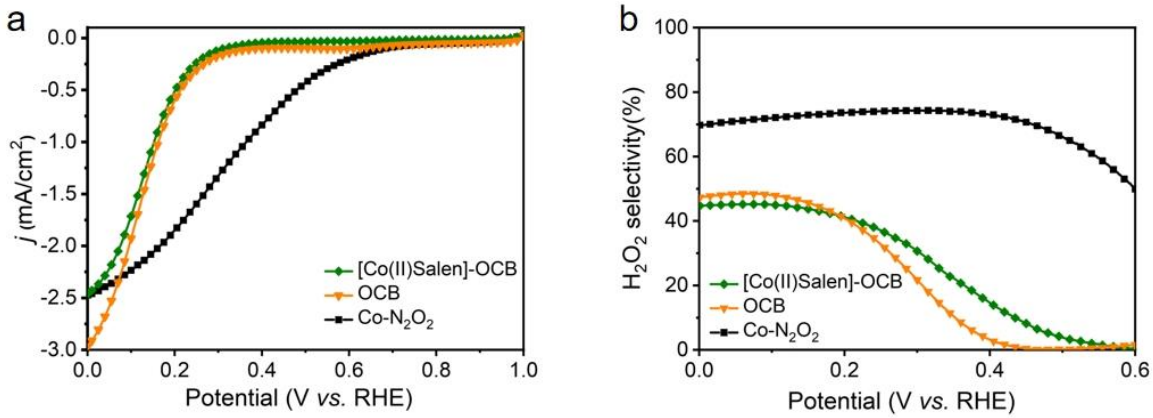

Fig. S7. (a) The ORR polarization curves and the ring electrode current in 0.1 M $HClO_4$ at 1600 rpm and (b) the calculated H_2O_2 selectivity of the OCB substrate, [Co(II)Salen]-OCB precursor, and Co-N_2O_2 catalyst.

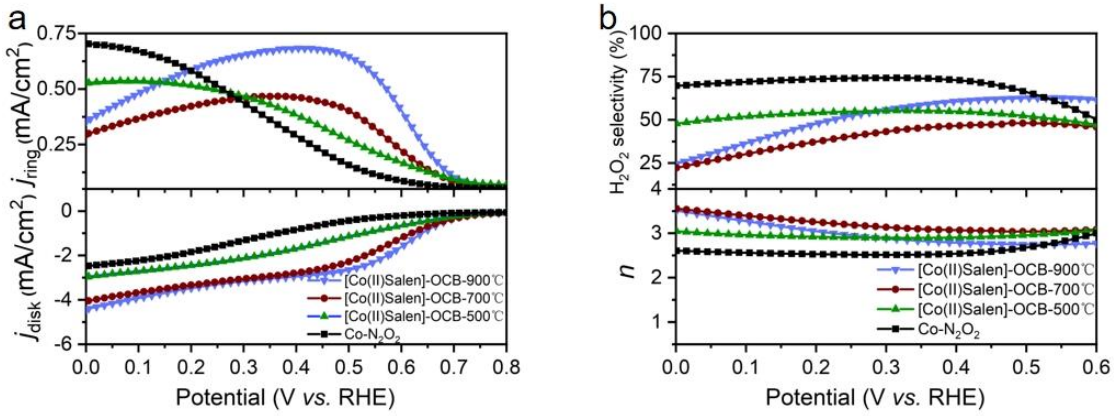

Fig. S8. (a) Linear sweep voltammetry curves recorded at 1600 rpm and a scan rate of 5 mV s^{-1} in O_2-saturated 0.1 M $HClO_4$, together with the detected H_2O_2 currents density on the ring electrode at a fixed potential of 1.3 V *vs*. RHE and (c) the calculated H_2O_2 selectivity and electron transfer number *n* during LSV scan of the [Co(II)Salen]-OCB-T °C catalysts (T=300, 500, 700, 900).

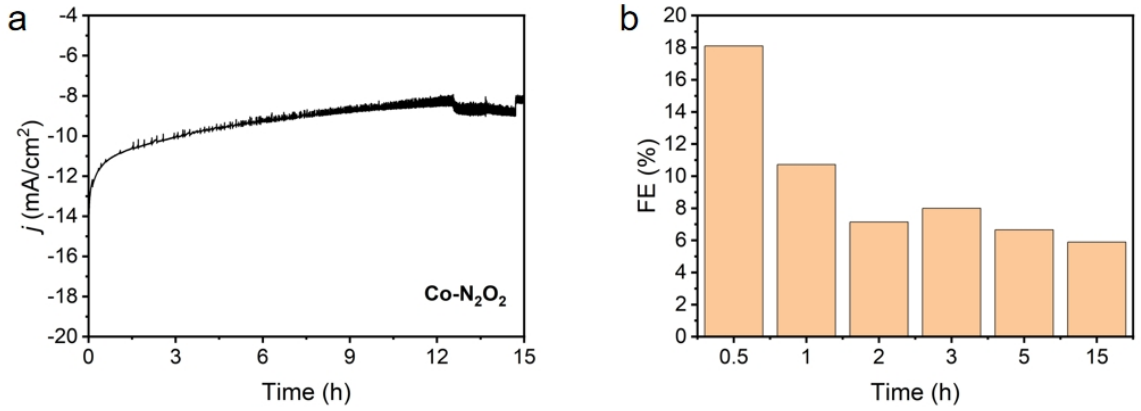

Fig. S9 (a) Stability measurement of Co-N_2O_2 catalyst at a constant potential of 0.35 V *vs.* RHE in 0.1M $HClO_4$ in an H-cell electrolyzer. (b) The calculated average FE of Co-N_2O_2 catalyst at a constant potential of 0.35 V *vs.* RHE in 0.1M $HClO_4$ in an H-cell electrolyzer.

Table S1. The element content of Co-N_2O_2, Co-N_4, Co-O_4 catalysts and OCB substrate analyzed by XPS.

Sample	Element Content (Atomic %)			
	Co	N	O	C
Co-N_2O_2	0.52	1.97	7.58	89.93
Co-N_4	0.43	3.87	2.75	91.65
Co-O_4	0.48	0.43	8.36	89.92
OCB	\	0.83	7.95	90.01

Table S2. The binding energy peak centers analyzed by XPS of different type N in the Co-N_2O_2 and Co-N_4 catalysts.

Sample	Binding Energy (eV)				
	Pyridinic-N	**Co-N_x**	**Pyrrolic-N**	**Graphitic-N**	**N-O**
Co-N_2O_2	398.5	399.6	401.1	402.1	405.0
Co-N_4	398.7	399.3	400.7	402.2	405.0

Table S3. The binding energy peak centers analyzed by XPS of different type O in the Co-N_2O_2 and Co-O_4 catalysts.

Sample	Binding Energy (eV)		
	C=O	**C-O-C**	**C-OH**
Co-N_2O_2	531.1	532.1	533.6
Co-O_4	531.3	532.4	533.9

Table S4. The scattering path, degeneracy, effective radius (Reff) and scattering type parameters in the crystallographic information file for the [Co(II)Salen], CoPc, and $Co(acac)_2$ molecule sample.

Sample	Path	Degeneracy	Reff	Type
[Co(II)Salen]	Co-N	2	1.841	Single scatterting
	Co-O	2	1.847	Single scatterting
CoPc	Co-N	4	1.915	Single scatterting
$Co(acac)_2$	Co-O	4	1.884	Single scatterting

Table S5. Co K-edge EXAFS curve-fitting parameters for the Co-N_2O_2, Co-N_4, Co-O_4, and [Co(II)Salen]-OCB-500 °C catalyst.

Sample	Path	CN	S_0^2	R(Å)	σ^2	ΔE_0 (eV)	R-factor
Co-N_2O_2	Co-N	2	0.746	1.80	0.01043	6.65	0.0166
	Co-O	2		1.85	0.00220	-1.60	
	Co-C	4.5		2.75	0.01103	0.56	
Co-N_4	Co-N	4	0.746	1.89	0.01069	3.20	0.0168
	Co-C	8		2.94	0.00809	3.26	
	Co-C	16		3.12	0.01004	5.37	
Co-O_4	Co-O	4.4	0.750	1.88	0.00336	2.10	0.0170
	Co-C	8.4		2.77	0.01764	7.48	
[Co(II)Salen]-OCB-500℃	Co-N	3.5	0.746	2.00	0.01156	1.57	0.0184
	Co-Co	1.1		2.58	0.01726	10	

CN: the coordination number.
S_0^2: the amplitude reduction factor (S_0^2 is determined by fitting EXAFS spectrum of Co foil).
R: the interatomic distance (bond length from center atom to coordination atom).
σ^2: Debye-Waller factor to evaluate thermal and static disorder.
ΔE_0: inner potential correction.
R-factor indicates the goodness of the fit.

Table S6. Raman spectra parameters of the OCB substrate, [Co(II)Salen]-OCB precursor, and Co-N_2O_2 catalyst.

Sample	Carbon type	Peak position	Peak height	I_D/I_G
Co-N_2O_2	D-band	1348.72	6731.24	1.09
	G-band	1588.85	6171.19	
[Co(II)Salen]-OCB	D-band	1347.97	7154.50	1.07
	G-band	1587.90	6690.25	
OCB	D-band	1331.84	6568.40	1.05
	G-band	1576.91	6229.45	