Supporting Information

Co nanoparticles encapsulated into N-doped carbon nanotube materials derived from new metal-organic frameworks for oxygen electrocatalysis

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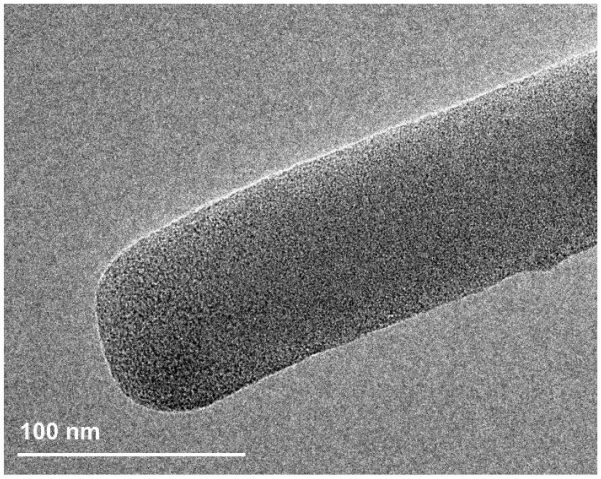

Fig. S1. TEM image of Co-MOF.

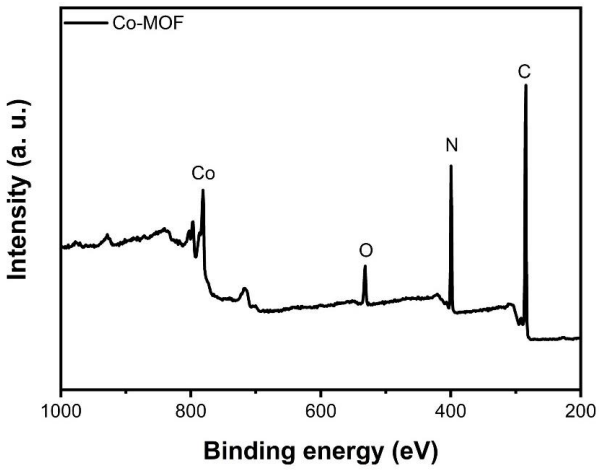

Fig. S2. Full survey XPS spectrum of Co-MOF.

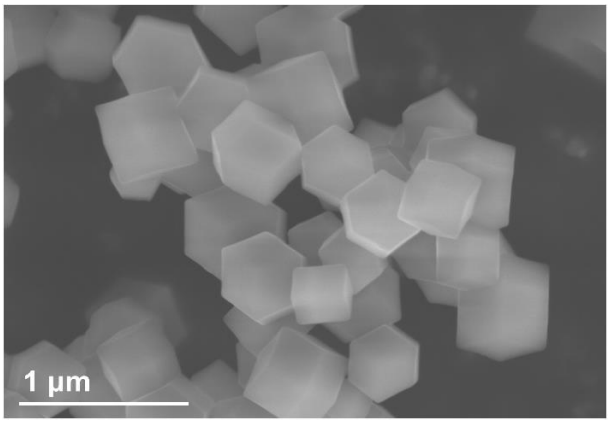

Fig. S3. SEM image of ZIF-67.

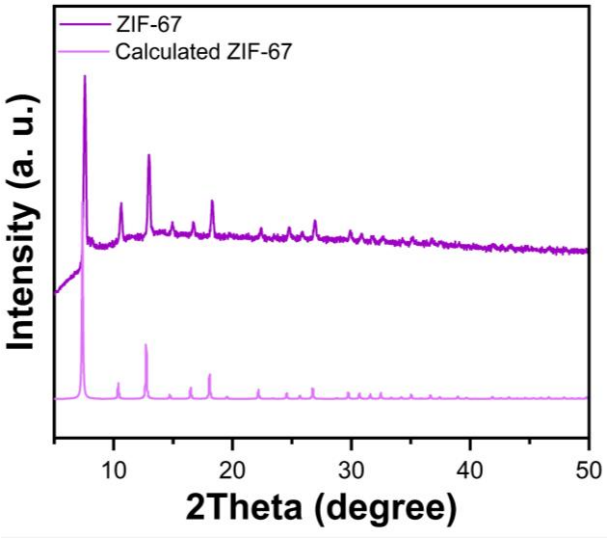

Fig. S4. XRD patterns of ZIF-67 and calculated ZIF-67.

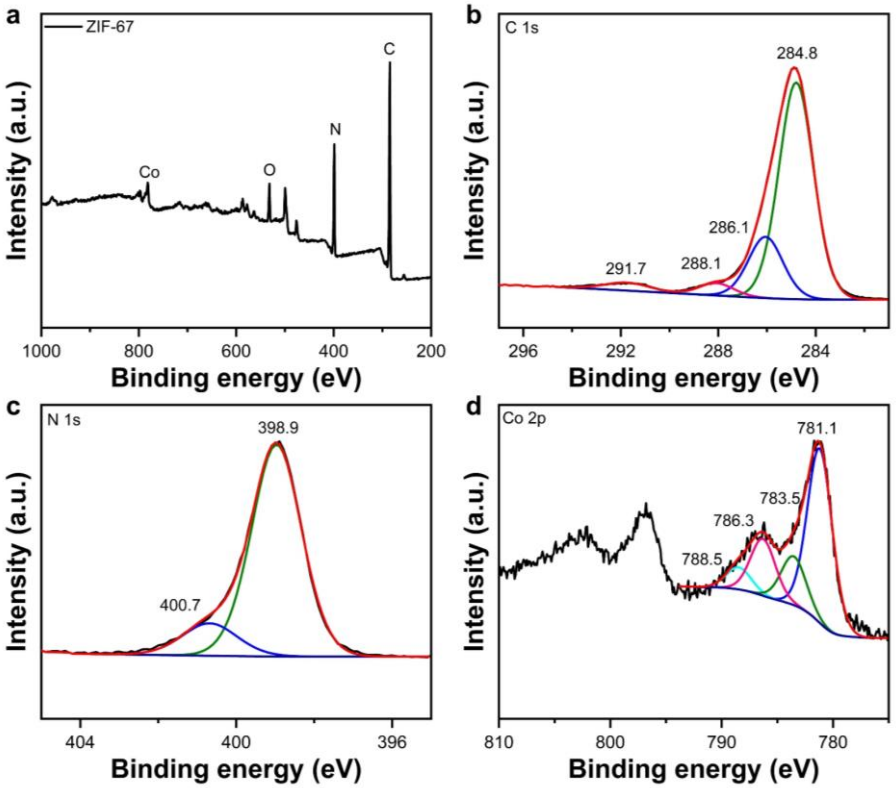

Fig. S5. Full survey XPS spectrum (a), XPS spectra of C 1s (b), N 1s (c), and Co 2p (d) for ZIF-67.

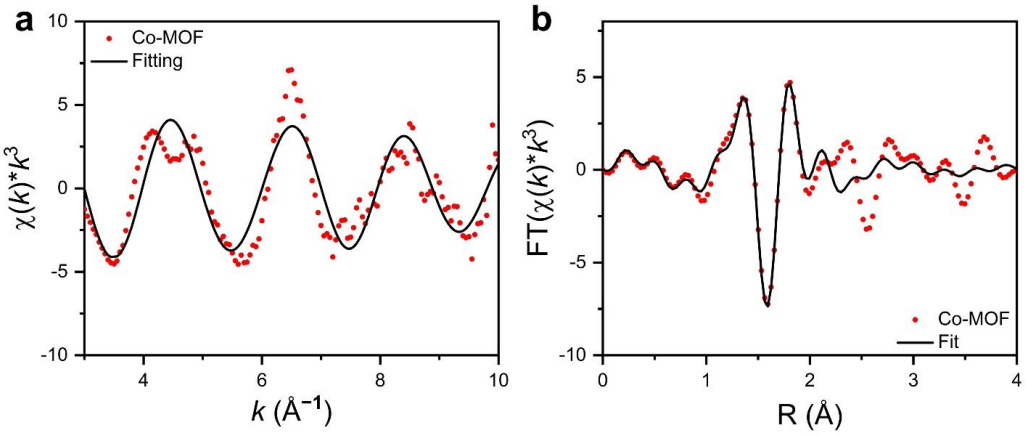

Fig. S6. (a) Corresponding Co K-edge k^3-weighted FT-EXAFS fitting curves of Co-MOF at R space (R imaginary) and (b) *k* space.

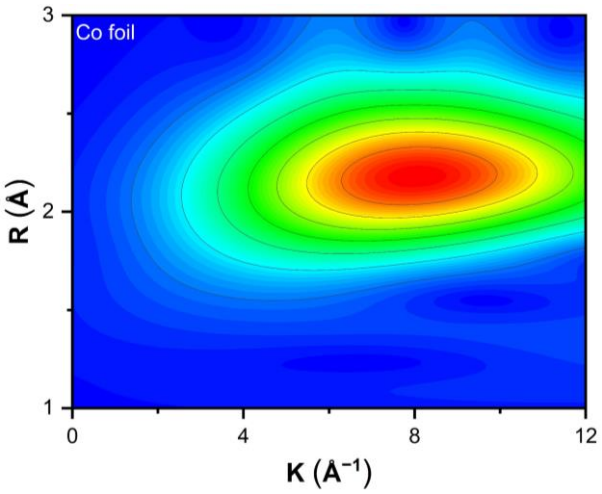

Fig. S7. Co K-edge WT-EXAFS contour plots of Co foil.

Fig. S8. Digital photo of ZIF-67.

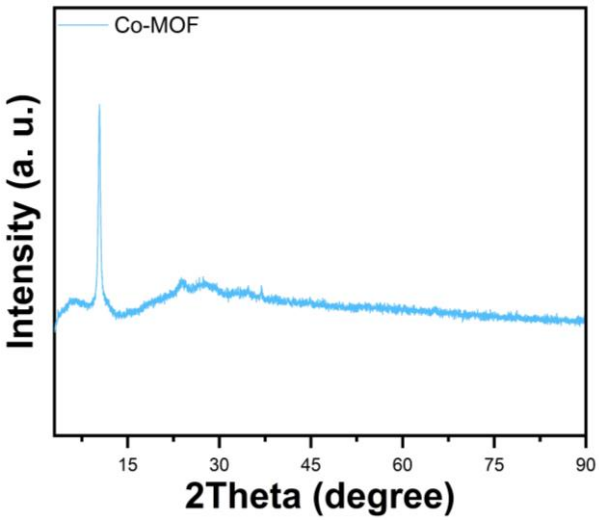

Fig. S9. XRD pattern of Co-MOF.

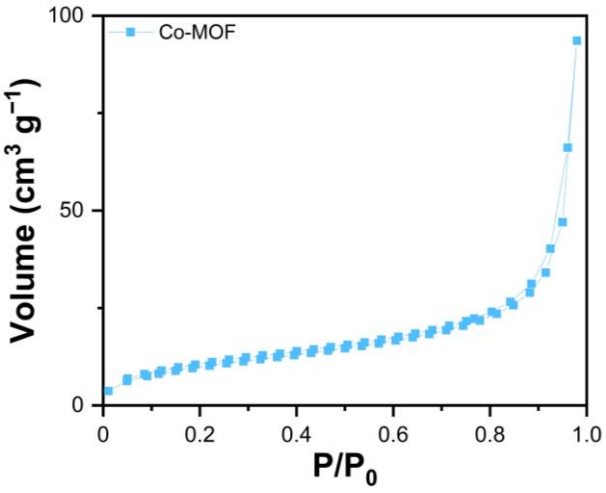

Fig. S10. N_2 adsorption/desorption isotherms of Co-MOF.

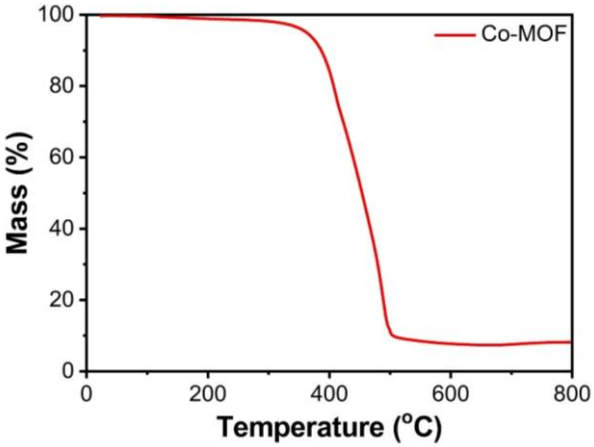

Fig. S11. The weight loss curve of Co-MOF.

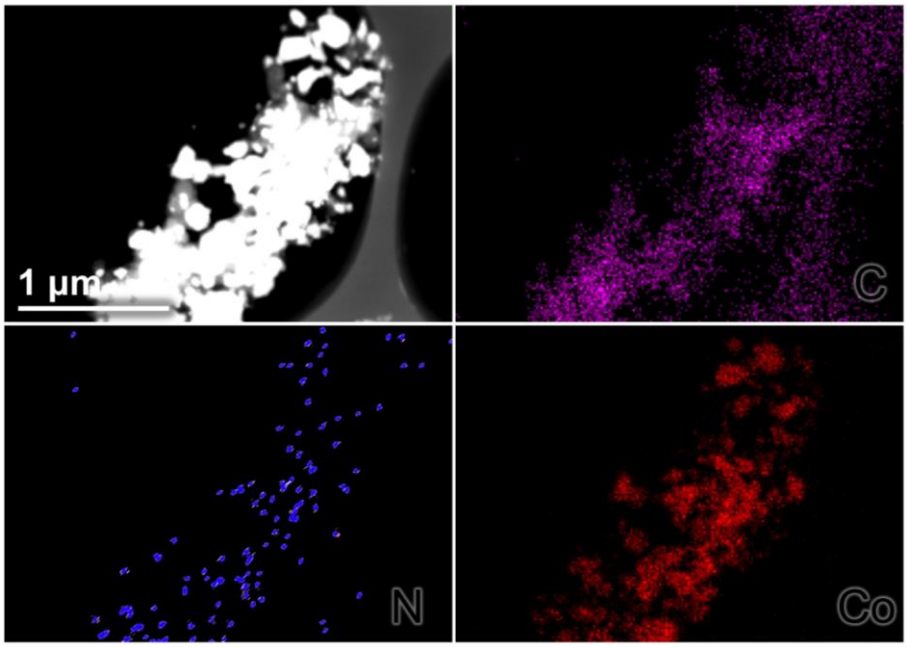

Fig. S12. HAADF-STEM image, and corresponding C, N, and Co elemental mappings of Co@N-CNT.

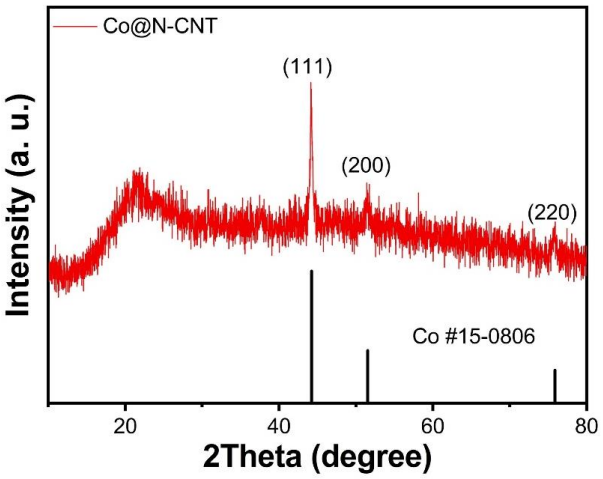

Fig. S13. XRD pattern of Co@N-CNT.

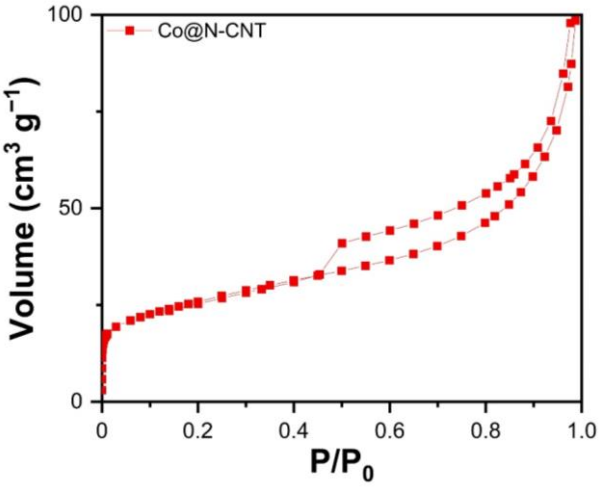

Fig. S14. N_2 adsorption/desorption isotherms of Co@N-CNT.

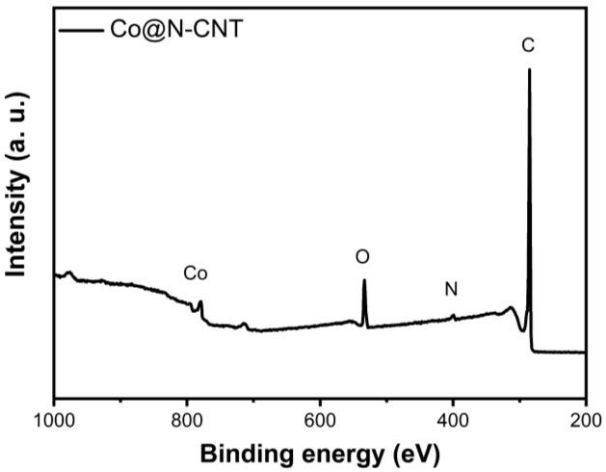

Fig. S15. Full survey XPS spectrum of Co@N-CNT.

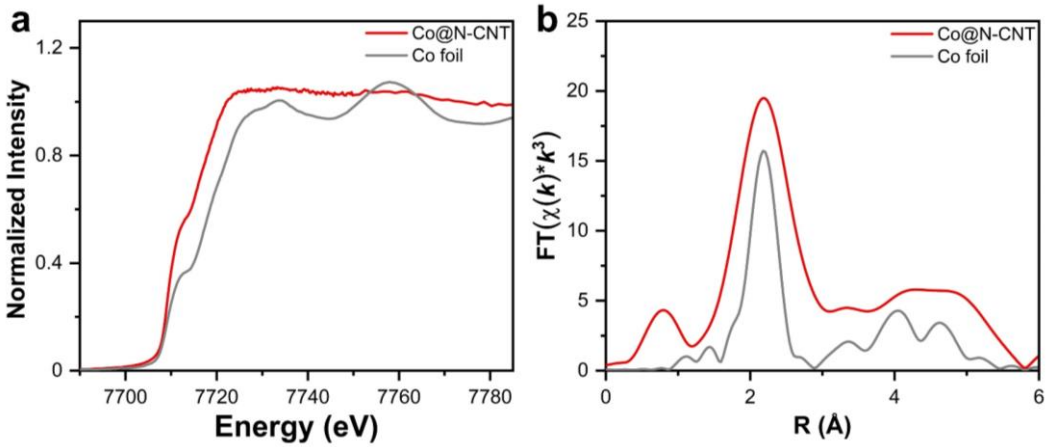

Fig. S16. (a) Normalized Co K-edge XANES and (b) k^3-weighted FT-EXAFS spectra (without phase correction) of Co@N-CNT and Co foil.

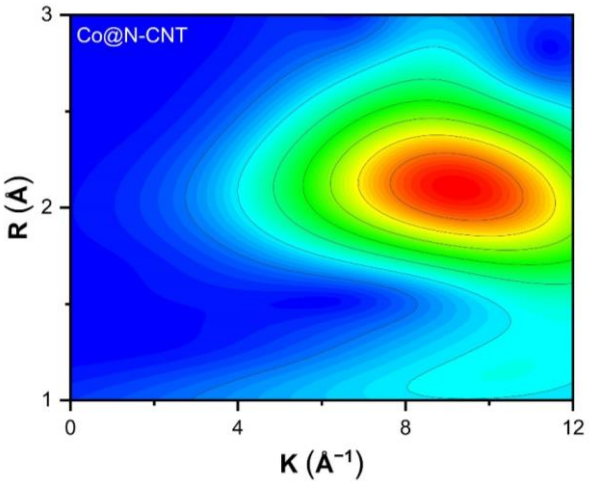

Fig. S17. Co K-edge WT-EXAFS contour plots of Co@N-CNT.

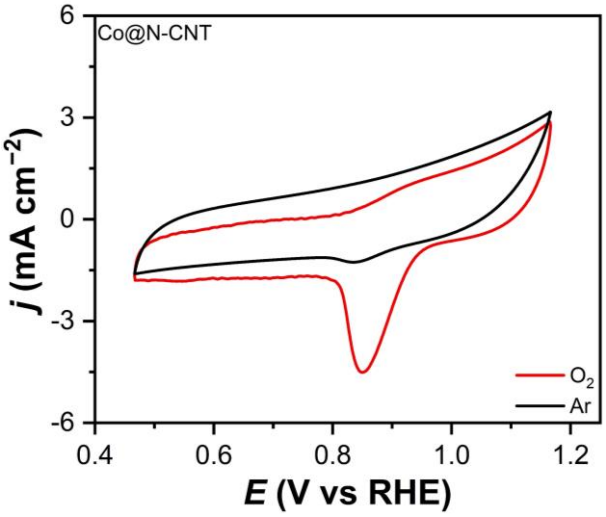

Fig. S18. CV data of Co@N-CNT measured in Ar and O_2-saturated 0.1 M KOH solutions.

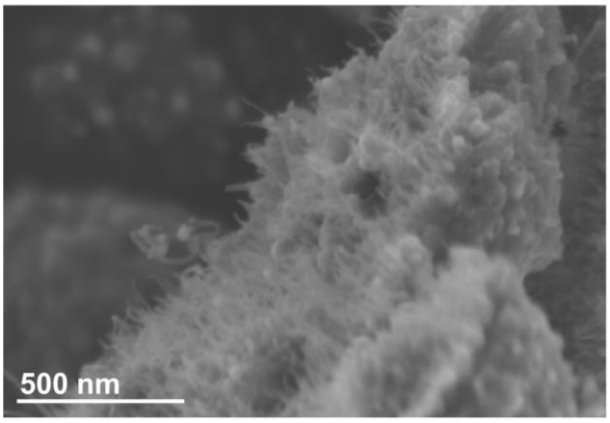

Fig. S19. SEM image of Co@N-CNT-800.

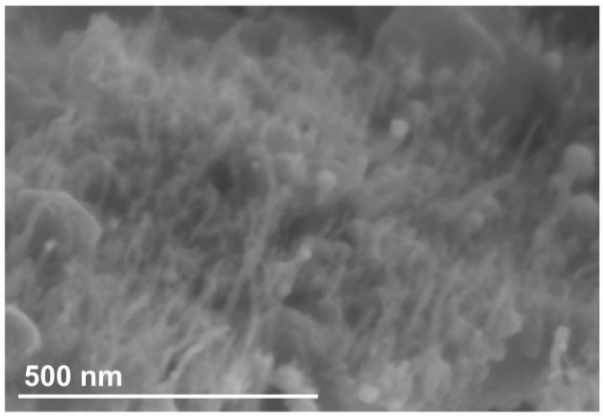

Fig. S20. SEM image of Co@N-CNT-1000

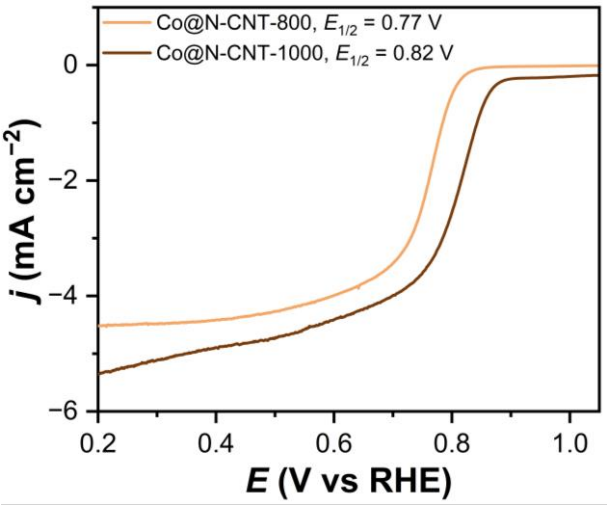

Fig. S21. ORR LSV curves of Co@N-CNT-800 and Co@N-CNT-1000.

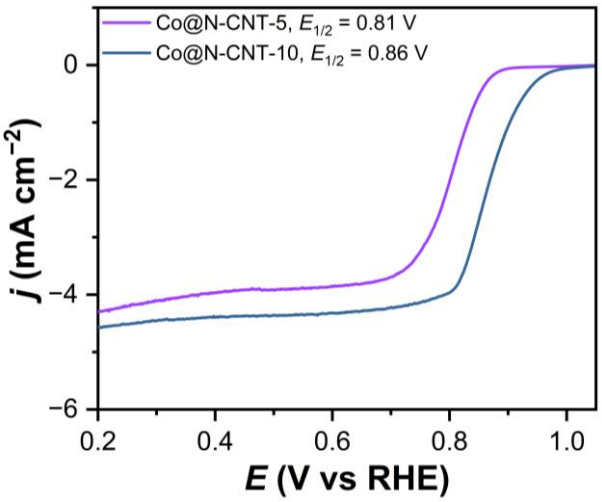

Fig. S22. ORR LSV curves of Co@N-CNT-5 and Co@N-CNT-10.

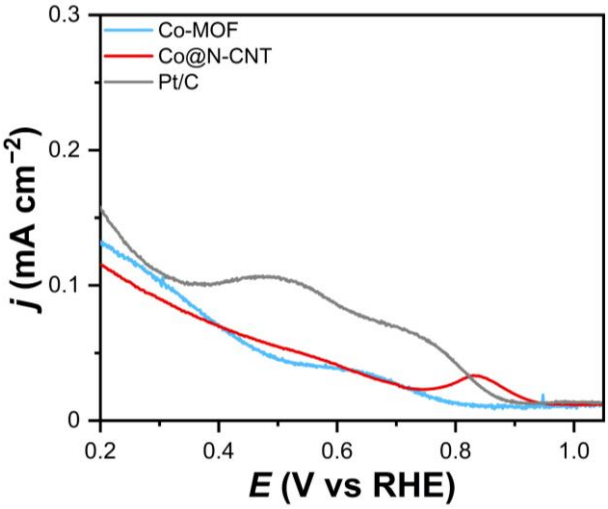

Fig. S23. ORR LSV data of Co-MOF, Co@N-CNT and Pt/C on the ring electrode.

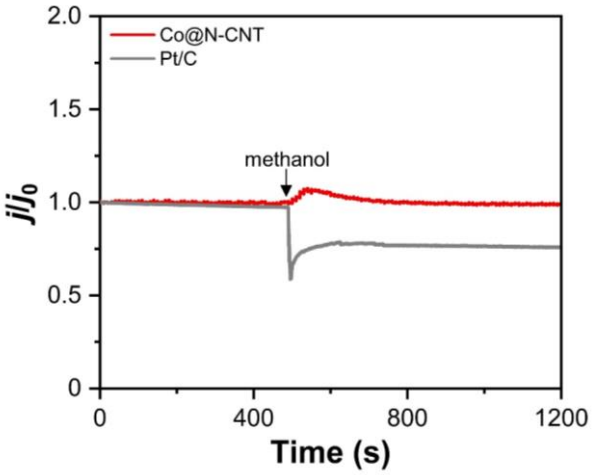

Fig. S24. Methanol resistance results of Co@N-CNT and Pt/C.

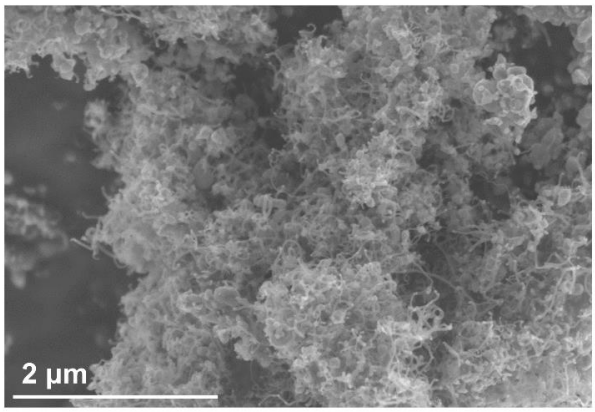

Fig. S25. SEM image of Co@N-CNT after ORR.

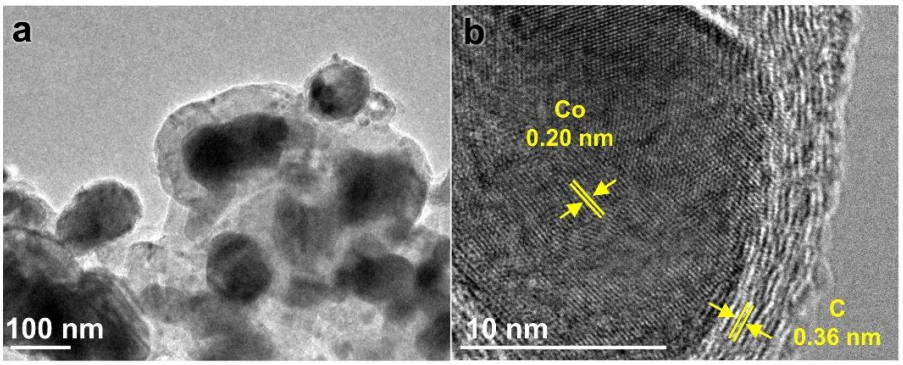

Fig. S26. TEM images of Co@N-CNT after ORR.

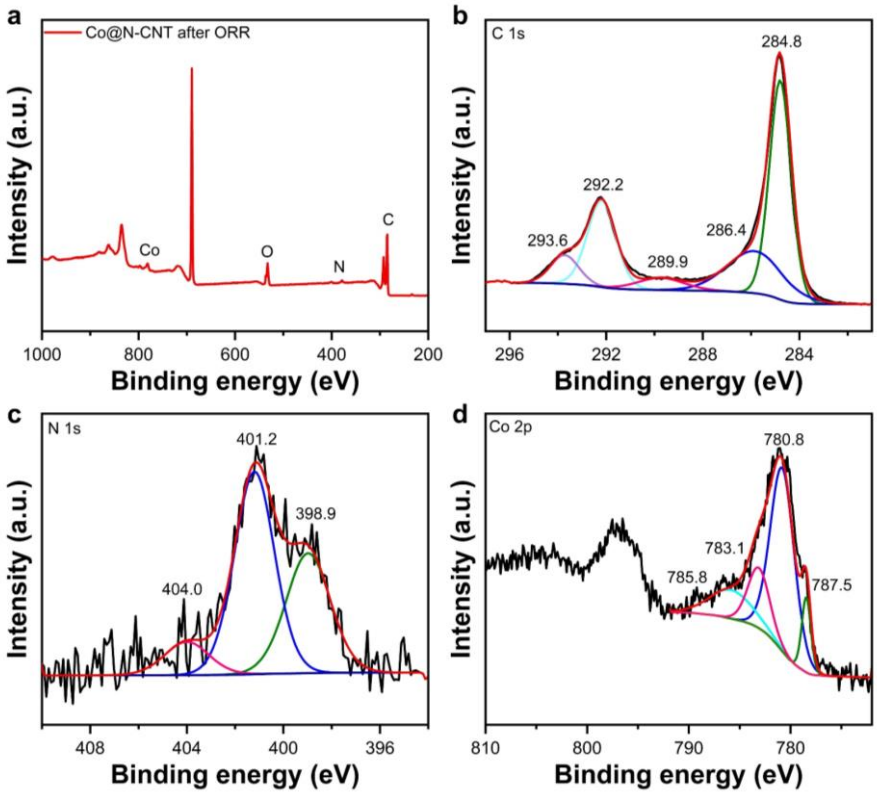

Fig. S27. Full survey XPS spectrum (a), XPS spectra of C 1s (b), N 1s (c) and Co 2p (d) for Co@N-CNT after ORR.

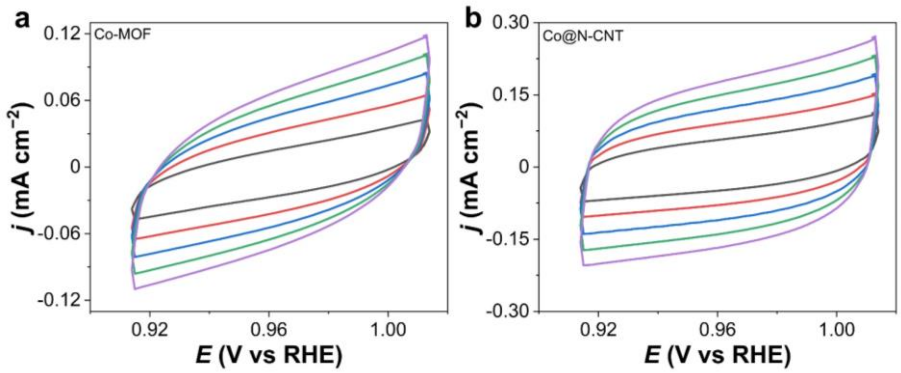

Fig. S28. CV data of Co-MOF and Co@N-CNT at 20, 40, 60, 80, and 100 mV s^{-1}.

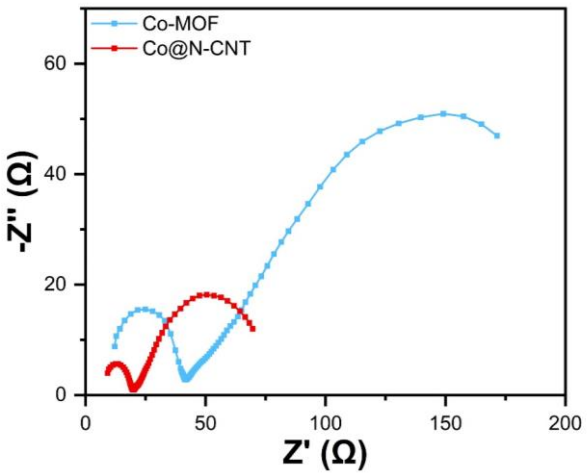

Fig. S29. Nyquist plots of Co-MOF and Co@N-CNT.

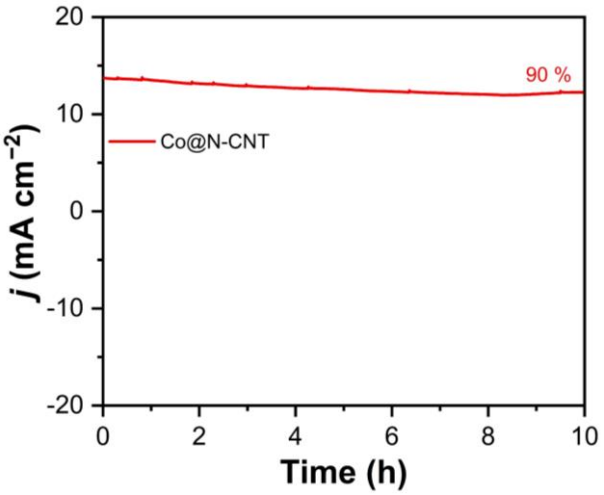

Fig. S30. Stability test of Co@N-CNT measured in a 1.0 M KOH solution.

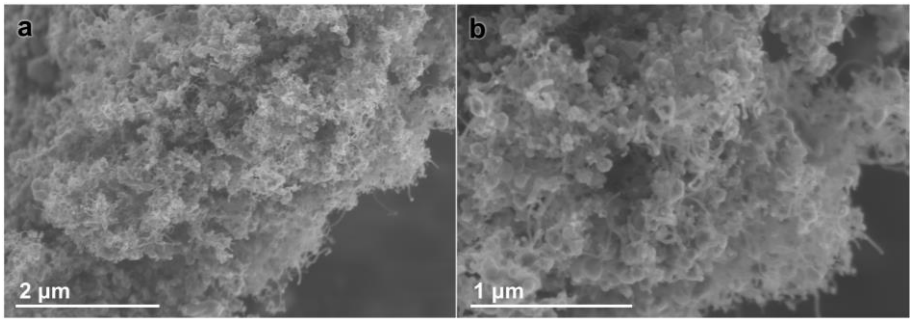

Fig. S31. SEM images of Co@N-CNT after OER.

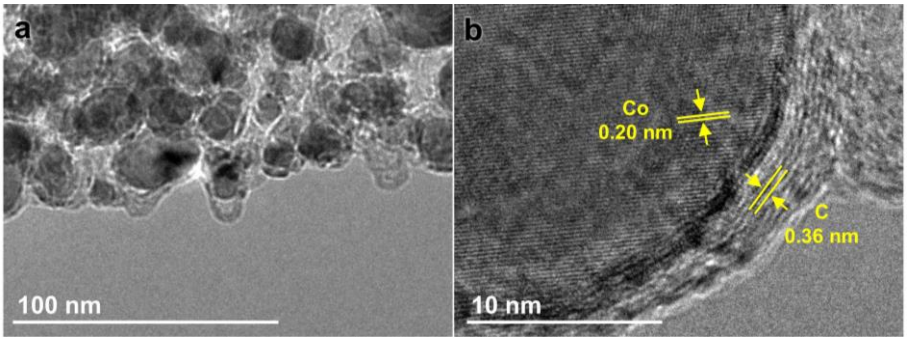

Fig. S32. TEM images of Co@N-CNT after OER.

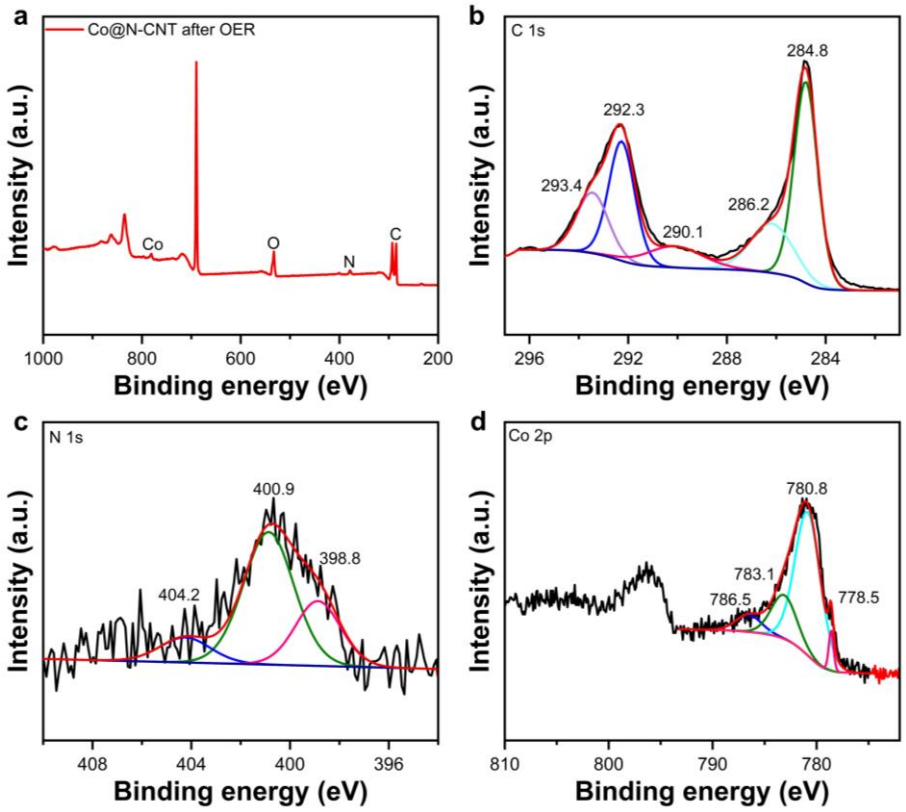

Fig. S33. Full survey XPS spectrum (a), XPS spectra of C 1s (b), N 1s (c), and Co 2p (d) for Co@N-CNT after OER.

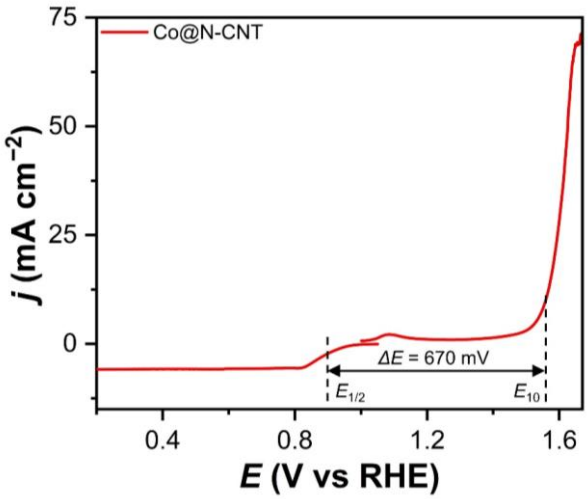

Fig. S34. ORR/OER LSV data of Co@N-CNT.

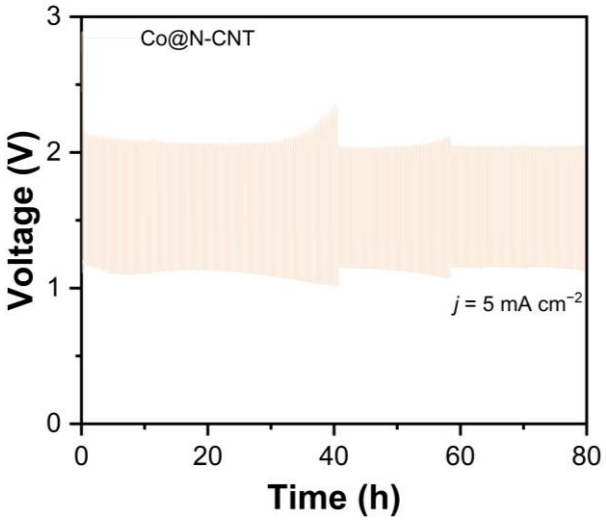

Fig. S35. Stability test at j = 5 mA cm^{-2} by a Zn-air battery assembled with Co@N-CNT.

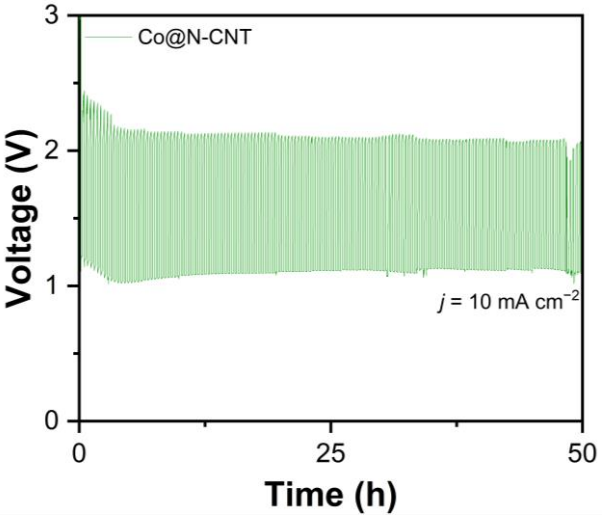

Fig. S36. Stability test at j = 10 mA cm^{-2} by a Zn-air battery assembled with Co@N-CNT.

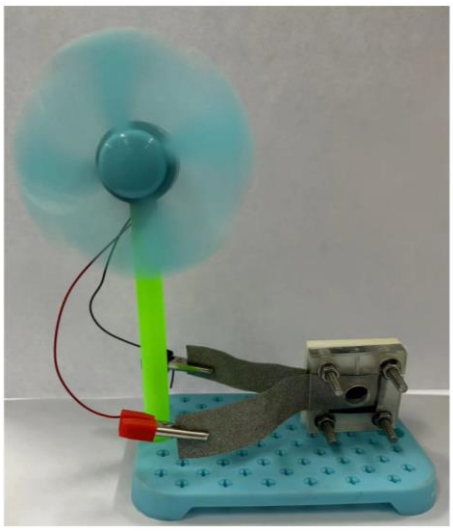

Fig. S37. A running toy fan powered by a Zn-air battery constructed with Co@N-CNT.

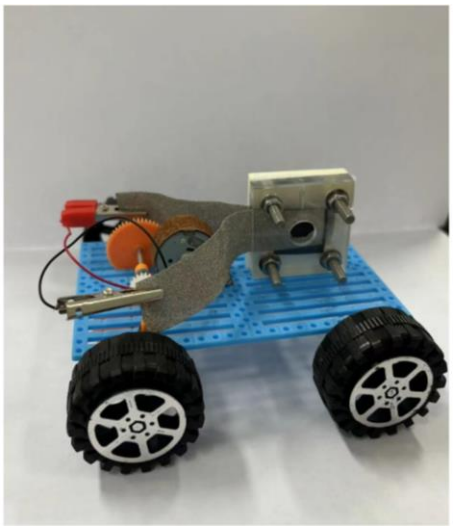

Fig. S38. A toy car powered by a Zn-air battery constructed with Co@N-CNT.

Table S1. The atomic proportions of Co-MOF and ZIF-67 given in XPS.

Elements	Atomic %	
	Co-MOF	**ZIF-67**
C	66.36	69.53
Co	6.19	2.13
N	21.59	19.97

Table S2. Comparison of ORR and OER performance of Co@N-CNT and other Co-based catalysts.

Catalysts	ORR $E_{1/2}$ (V)	OER η (mV, j_{10})	References
Co@N-CNT	**0.88**	**320**	**This work**
Co_4-Co-MOF	0.83	357	1
Co_4N/CoNC	0.833	270	2
Onion-like carbon/Co-N-C	0.855	344	3
$NiCo_{1.8}Fe_{0.2}O_4$@N-carbon	0.86	270	4
Co corroles@CNT	0.80	450	5
Co_3O_{4-X} doped graphene	0.829	327	6
Co/N-boron graphene	0.867	365	7
PVP-ZIF-67-4	0.85	315	8
$Ni_xCo_{9-x}S_8$@ N, S co-doped carbon	0.926	289	9
Co_3O_4/RuO_2/carbon sheets	0.90	290	10
Co-N-C@HCNT	0.86	385	11
CoFe/Co-N-C	0.86	380	12
Zn_{20}Co-N-C	0.915	-	13
Co@N-doped graphene	0.85	-	14
N/P-C-CoP-850	0.825	306	15
MoC/Co-N-C-600	0.865	370	16
A-Co-N-C	0.884	334	17
NiS_2@Co-N-C/nanoarchitecture	0.80	300	18
Pt_{SA}-PtCo NCs/N-CNTs-900	0.86	252	19
Co-single-atom/N-C/reduced graphene oxide	0.84	-	20

Table S3. Comparison of peak power densities of Zn-air batteries constructed with Co@N-CNT and other reported catalysts.

Catalysts	**Voltage gap (V)**	**Peak power density ($mW\ cm^{-2}$)**	**References**
Co@N-CNT	**0.82**	**235**	**This work**
Co-N-C	0.85	203	21
Co-porous organic polymers	0.91	207.1	22
Onion-like carbon/Co-N-C	0.80	238	3
Co_{SAs}@NC-920	0.812	166	23
NCo@CNT-nanofiber700	0.80	220	24
A-Co-N-C	0.85	240	17
Co-N_{4-x}-C_x	0.80	184	25
$(Co, Fe)_3N$	0.85	234	26
$Fe_{atomic\ clusters}$@N-C	0.80	171.5	27
Co-FNC	0.90	246	28
HfCo-NC	-	184	29
Co/N, S-C	0.82	173.1	30
Cl−Co−N_4	0.80	176.6	31

Atomic coordinates of cobalt cluster cell models.

	x	y	z	Occ.	U	Site	Sym.
1 Co Co1	0.51837	0.49721	0.52594	1.000	0.000	1a	1
2 Co Co2	0.51837	0.65019	0.59354	1.000	0.000	1a	1
3 Co Co3	0.69501	0.58554	0.59354	1.000	0.000	1a	1
4 Co Co4	0.69501	0.73852	0.52594	1.000	0.000	1a	1
5 Co Co5	0.51837	0.34424	0.45835	1.000	0.000	1a	1
6 Co Co6	0.34172	0.40889	0.45835	1.000	0.000	1a	1
7 Co Co7	0.51837	0.65019	0.45835	1.000	0.000	1a	1
8 Co Co8	0.69501	0.58554	0.45835	1.000	0.000	1a	1
9 Co Co9	0.34172	0.25591	0.52594	1.000	0.000	1a	1
10 Co Co10	0.51837	0.34424	0.59354	1.000	0.000	1a	1
11 Co Co11	0.69501	0.43256	0.52594	1.000	0.000	1a	1
12 Co Co12	0.34172	0.40889	0.59354	1.000	0.000	1a	1
13 Co Co13	0.34172	0.56187	0.52594	1.000	0.000	1a	1

Atomic coordinates of Co@CNT cell models.

		x	y	z	Occ.	U	Site	Sym.
1 C	C1	0.91886	0.75352	0.00527	1.000	0.000	1a	1
2 C	C2	0.90068	0.81933	0.04725	1.000	0.000	1a	1
3 C	C3	0.77306	0.92173	0.00598	1.000	0.000	1a	1
4 C	C4	0.83473	0.89610	0.04753	1.000	0.000	1a	1
5 C	C5	0.35353	0.77515	0.00565	1.000	0.000	1a	1
6 C	C6	0.66899	0.92885	0.00619	1.000	0.000	1a	1
7 C	C7	0.58221	0.90391	0.04799	1.000	0.000	1a	1
8 C	C8	0.24406	0.66897	0.00538	1.000	0.000	1a	1
9 C	C9	0.17942	0.58478	0.04735	1.000	0.000	1a	1
10 C	C10	0.43925	0.83545	0.04774	1.000	0.000	1a	1
11 C	C11	0.08525	0.35644	0.00525	1.000	0.000	1a	1
12 C	C12	0.10659	0.44154	0.04717	1.000	0.000	1a	1
13 C	C13	0.22627	0.07821	0.00594	1.000	0.000	1a	1
14 C	C14	0.08028	0.24631	0.00529	1.000	0.000	1a	1
15 C	C15	0.09876	0.18062	0.04724	1.000	0.000	1a	1
16 C	C16	0.33024	0.07092	0.00620	1.000	0.000	1a	1
17 C	C17	0.41710	0.09599	0.04799	1.000	0.000	1a	1
18 C	C18	0.16470	0.10388	0.04753	1.000	0.000	1a	1
19 C	C19	0.64558	0.22474	0.00559	1.000	0.000	1a	1
20 C	C20	0.56000	0.16454	0.04772	1.000	0.000	1a	1
21 C	C21	0.91384	0.64337	0.00522	1.000	0.000	1a	1
22 C	C22	0.75493	0.33103	0.00536	1.000	0.000	1a	1
23 C	C23	0.81983	0.41515	0.04732	1.000	0.000	1a	1
24 C	C24	0.89272	0.55840	0.04715	1.000	0.000	1a	1

25 C	C25	0.91522	0.76137	0.09457	1.000	0.000	1a	1
26 C	C26	0.89609	0.81256	0.14223	1.000	0.000	1a	1
27 C	C27	0.77806	0.91084	0.09521	1.000	0.000	1a	1
28 C	C28	0.82635	0.88630	0.14249	1.000	0.000	1a	1
29 C	C29	0.36566	0.77939	0.09510	1.000	0.000	1a	1
30 C	C30	0.65316	0.91401	0.09540	1.000	0.000	1a	1
31 C	C31	0.58142	0.89117	0.14283	1.000	0.000	1a	1
32 C	C32	0.23697	0.65585	0.09493	1.000	0.000	1a	1
33 C	C33	0.18861	0.58323	0.14233	1.000	0.000	1a	1
34 C	C34	0.43738	0.82461	0.14269	1.000	0.000	1a	1
35 C	C35	0.08957	0.36784	0.09453	1.000	0.000	1a	1
36 C	C36	0.11480	0.43932	0.14223	1.000	0.000	1a	1
37 C	C37	0.22129	0.08909	0.09521	1.000	0.000	1a	1
38 C	C38	0.08424	0.23857	0.09459	1.000	0.000	1a	1
39 C	C39	0.10329	0.18731	0.14225	1.000	0.000	1a	1
40 C	C40	0.34630	0.08613	0.09540	1.000	0.000	1a	1
41 C	C41	0.41810	0.10891	0.14281	1.000	0.000	1a	1
42 C	C42	0.17300	0.11351	0.14250	1.000	0.000	1a	1
43 C	C43	0.63374	0.22057	0.09506	1.000	0.000	1a	1
44 C	C44	0.56213	0.17512	0.14267	1.000	0.000	1a	1
45 C	C45	0.90997	0.63210	0.09451	1.000	0.000	1a	1
46 C	C46	0.76244	0.34406	0.09488	1.000	0.000	1a	1
47 C	C47	0.81085	0.41665	0.14229	1.000	0.000	1a	1
48 C	C48	0.88466	0.56055	0.14218	1.000	0.000	1a	1
49 C	C49	0.91265	0.75997	0.18956	1.000	0.000	1a	1
50 C	C50	0.89395	0.81096	0.23694	1.000	0.000	1a	1

51 C	C51	0.77412	0.90403	0.18979	1.000	0.000	1a	1
52 C	C52	0.82398	0.88408	0.23700	1.000	0.000	1a	1
53 C	C53	0.36618	0.77440	0.18984	1.000	0.000	1a	1
54 C	C54	0.65086	0.90662	0.18990	1.000	0.000	1a	1
55 C	C55	0.58071	0.88861	0.23694	1.000	0.000	1a	1
56 C	C56	0.23984	0.65244	0.18977	1.000	0.000	1a	1
57 C	C57	0.18961	0.58184	0.23695	1.000	0.000	1a	1
58 C	C58	0.43697	0.82171	0.23700	1.000	0.000	1a	1
59 C	C59	0.09303	0.36797	0.18954	1.000	0.000	1a	1
60 C	C60	0.11546	0.43827	0.23687	1.000	0.000	1a	1
61 C	C61	0.22538	0.09585	0.18980	1.000	0.000	1a	1
62 C	C62	0.08665	0.23981	0.18960	1.000	0.000	1a	1
63 C	C63	0.10545	0.18879	0.23697	1.000	0.000	1a	1
64 C	C64	0.34874	0.09334	0.18992	1.000	0.000	1a	1
65 C	C65	0.41899	0.11111	0.23692	1.000	0.000	1a	1
66 C	C66	0.17553	0.11571	0.23702	1.000	0.000	1a	1
67 C	C67	0.63346	0.22523	0.18981	1.000	0.000	1a	1
68 C	C68	0.56279	0.17775	0.23700	1.000	0.000	1a	1
69 C	C69	0.90645	0.63188	0.18950	1.000	0.000	1a	1
70 C	C70	0.75964	0.34740	0.18973	1.000	0.000	1a	1
71 C	C71	0.80993	0.41810	0.23691	1.000	0.000	1a	1
72 C	C72	0.88414	0.56162	0.23682	1.000	0.000	1a	1
73 C	C73	0.90938	0.75849	0.28429	1.000	0.000	1a	1
74 C	C74	0.88737	0.80752	0.33126	1.000	0.000	1a	1
75 C	C75	0.77310	0.90444	0.28411	1.000	0.000	1a	1
76 C	C76	0.81905	0.88124	0.33126	1.000	0.000	1a	1

77 C	C77	0.36691	0.77277	0.28428	1.000	0.000	1a	1
78 C	C78	0.64992	0.90700	0.28417	1.000	0.000	1a	1
79 C	C79	0.57985	0.88737	0.33126	1.000	0.000	1a	1
80 C	C80	0.24092	0.65073	0.28431	1.000	0.000	1a	1
81 C	C81	0.19248	0.57985	0.33126	1.000	0.000	1a	1
82 C	C82	0.43782	0.81905	0.33126	1.000	0.000	1a	1
83 C	C83	0.09450	0.36789	0.28415	1.000	0.000	1a	1
84 C	C84	0.11876	0.43782	0.33126	1.000	0.000	1a	1
85 C	C85	0.22676	0.09554	0.28408	1.000	0.000	1a	1
86 C	C86	0.09032	0.24137	0.28432	1.000	0.000	1a	1
87 C	C87	0.11263	0.19248	0.33126	1.000	0.000	1a	1
88 C	C88	0.34990	0.09291	0.28417	1.000	0.000	1a	1
89 C	C89	0.42015	0.11263	0.33126	1.000	0.000	1a	1
90 C	C90	0.18095	0.11876	0.33126	1.000	0.000	1a	1
91 C	C91	0.63295	0.22702	0.28425	1.000	0.000	1a	1
92 C	C92	0.56218	0.18095	0.33126	1.000	0.000	1a	1
93 C	C93	0.90525	0.63203	0.28412	1.000	0.000	1a	1
94 C	C94	0.75882	0.34926	0.28429	1.000	0.000	1a	1
95 C	C95	0.80752	0.42015	0.33126	1.000	0.000	1a	1
96 C	C96	0.88124	0.56218	0.33126	1.000	0.000	1a	1
97 C	C97	0.90431	0.75601	0.37858	1.000	0.000	1a	1
98 C	C98	0.88737	0.80752	0.42590	1.000	0.000	1a	1
99 C	C99	0.76975	0.90120	0.37858	1.000	0.000	1a	1
100 C	C100	0.81905	0.88124	0.42590	1.000	0.000	1a	1
101 C	C101	0.36855	0.76975	0.37858	1.000	0.000	1a	1
102 C	C102	0.64830	0.90431	0.37858	1.000	0.000	1a	1

103 C	C103	0.57985	0.88737	0.42590	1.000	0.000	1a	1
104 C	C104	0.24399	0.64830	0.37858	1.000	0.000	1a	1
105 C	C105	0.19248	0.57985	0.42590	1.000	0.000	1a	1
106 C	C106	0.43782	0.81905	0.42590	1.000	0.000	1a	1
107 C	C107	0.09880	0.36855	0.37858	1.000	0.000	1a	1
108 C	C108	0.11876	0.43782	0.42590	1.000	0.000	1a	1
109 C	C109	0.23025	0.09880	0.37858	1.000	0.000	1a	1
110 C	C110	0.09569	0.24399	0.37858	1.000	0.000	1a	1
111 C	C111	0.11263	0.19248	0.42590	1.000	0.000	1a	1
112 C	C112	0.35170	0.09569	0.37858	1.000	0.000	1a	1
113 C	C113	0.42015	0.11263	0.42590	1.000	0.000	1a	1
114 C	C114	0.18095	0.11876	0.42590	1.000	0.000	1a	1
115 C	C115	0.63145	0.23025	0.37858	1.000	0.000	1a	1
116 C	C116	0.56218	0.18095	0.42590	1.000	0.000	1a	1
117 C	C117	0.90120	0.63145	0.37858	1.000	0.000	1a	1
118 C	C118	0.75601	0.35170	0.37858	1.000	0.000	1a	1
119 C	C119	0.80752	0.42015	0.42590	1.000	0.000	1a	1
120 C	C120	0.88124	0.56218	0.42590	1.000	0.000	1a	1
121 C	C121	0.90431	0.75601	0.47322	1.000	0.000	1a	1
122 C	C122	0.88737	0.80752	0.52055	1.000	0.000	1a	1
123 C	C123	0.76975	0.90120	0.47322	1.000	0.000	1a	1
124 C	C124	0.81905	0.88124	0.52055	1.000	0.000	1a	1
125 C	C125	0.36855	0.76975	0.47322	1.000	0.000	1a	1
126 C	C126	0.64830	0.90431	0.47322	1.000	0.000	1a	1
127 C	C127	0.57985	0.88737	0.52055	1.000	0.000	1a	1
128 C	C128	0.24399	0.64830	0.47322	1.000	0.000	1a	1

129 C	C129	0.19248	0.57985	0.52055	1.000	0.000	1a	1
130 C	C130	0.43782	0.81905	0.52055	1.000	0.000	1a	1
131 C	C131	0.09880	0.36855	0.47322	1.000	0.000	1a	1
132 C	C132	0.11876	0.43782	0.52055	1.000	0.000	1a	1
133 C	C133	0.23025	0.09880	0.47322	1.000	0.000	1a	1
134 C	C134	0.09569	0.24399	0.47322	1.000	0.000	1a	1
135 C	C135	0.11263	0.19248	0.52055	1.000	0.000	1a	1
136 C	C136	0.35170	0.09569	0.47322	1.000	0.000	1a	1
137 C	C137	0.42015	0.11263	0.52055	1.000	0.000	1a	1
138 C	C138	0.18095	0.11876	0.52055	1.000	0.000	1a	1
139 C	C139	0.63145	0.23025	0.47322	1.000	0.000	1a	1
140 C	C140	0.56218	0.18095	0.52055	1.000	0.000	1a	1
141 C	C141	0.90120	0.63145	0.47322	1.000	0.000	1a	1
142 C	C142	0.75601	0.35170	0.47322	1.000	0.000	1a	1
143 C	C143	0.80752	0.42015	0.52055	1.000	0.000	1a	1
144 C	C144	0.88124	0.56218	0.52055	1.000	0.000	1a	1
145 C	C145	0.90431	0.75601	0.56787	1.000	0.000	1a	1
146 C	C146	0.88737	0.80752	0.61519	1.000	0.000	1a	1
147 C	C147	0.76975	0.90120	0.56787	1.000	0.000	1a	1
148 C	C148	0.81905	0.88124	0.61519	1.000	0.000	1a	1
149 C	C149	0.36855	0.76975	0.56787	1.000	0.000	1a	1
150 C	C150	0.64830	0.90431	0.56787	1.000	0.000	1a	1
151 C	C151	0.57985	0.88737	0.61519	1.000	0.000	1a	1
152 C	C152	0.24399	0.64830	0.56787	1.000	0.000	1a	1
153 C	C153	0.19248	0.57985	0.61519	1.000	0.000	1a	1
154 C	C154	0.43782	0.81905	0.61519	1.000	0.000	1a	1

155 C	C155	0.09880	0.36855	0.56787	1.000	0.000	1a	1
156 C	C156	0.11876	0.43782	0.61519	1.000	0.000	1a	1
157 C	C157	0.23025	0.09880	0.56787	1.000	0.000	1a	1
158 C	C158	0.09569	0.24399	0.56787	1.000	0.000	1a	1
159 C	C159	0.11263	0.19248	0.61519	1.000	0.000	1a	1
160 C	C160	0.35170	0.09569	0.56787	1.000	0.000	1a	1
161 C	C161	0.42015	0.11263	0.61519	1.000	0.000	1a	1
162 C	C162	0.18095	0.11876	0.61519	1.000	0.000	1a	1
163 C	C163	0.63145	0.23025	0.56787	1.000	0.000	1a	1
164 C	C164	0.56218	0.18095	0.61519	1.000	0.000	1a	1
165 C	C165	0.90120	0.63145	0.56787	1.000	0.000	1a	1
166 C	C166	0.75601	0.35170	0.56787	1.000	0.000	1a	1
167 C	C167	0.80752	0.42015	0.61519	1.000	0.000	1a	1
168 C	C168	0.88124	0.56218	0.61519	1.000	0.000	1a	1
169 Co	Co169	0.50882	0.49988	0.52594	1.000	0.000	1a	1
170 Co	Co170	0.50882	0.65286	0.59354	1.000	0.000	1a	1
171 Co	Co171	0.68547	0.58820	0.59354	1.000	0.000	1a	1
172 Co	Co172	0.68547	0.74118	0.52594	1.000	0.000	1a	1
173 Co	Co173	0.50882	0.34690	0.45835	1.000	0.000	1a	1
174 Co	Co174	0.33218	0.41156	0.45835	1.000	0.000	1a	1
175 Co	Co175	0.50882	0.65286	0.45835	1.000	0.000	1a	1
176 Co	Co176	0.68547	0.58820	0.45835	1.000	0.000	1a	1
177 Co	Co177	0.33218	0.25858	0.52594	1.000	0.000	1a	1
178 Co	Co178	0.50882	0.34690	0.59354	1.000	0.000	1a	1
179 Co	Co179	0.68547	0.43522	0.52594	1.000	0.000	1a	1
180 Co	Co180	0.33218	0.41156	0.59354	1.000	0.000	1a	1

181	Co	Co181	0.33218	0.56454	0.52594	1.000	0.000	1a		1

Atomic coordinates of Co@N-CNT cell models.

		x	y	z	Occ.	U	Site	Sym.
1 C	C1	0.91918	0.75309	0.00523	1.000	0.000	1a	1
2 C	C2	0.90002	0.81820	0.04726	1.000	0.000	1a	1
3 C	C3	0.77364	0.92173	0.00596	1.000	0.000	1a	1
4 C	C4	0.83469	0.89520	0.04750	1.000	0.000	1a	1
5 C	C5	0.35423	0.77497	0.00559	1.000	0.000	1a	1
6 C	C6	0.67012	0.92988	0.00626	1.000	0.000	1a	1
7 C	C7	0.58277	0.90365	0.04799	1.000	0.000	1a	1
8 C	C8	0.24418	0.66934	0.00541	1.000	0.000	1a	1
9 C	C9	0.18047	0.58445	0.04738	1.000	0.000	1a	1
10 C	C10	0.44022	0.83498	0.04769	1.000	0.000	1a	1
11 C	C11	0.08443	0.35575	0.00533	1.000	0.000	1a	1
12 C	C12	0.10752	0.44155	0.04722	1.000	0.000	1a	1
13 C	C13	0.22662	0.07805	0.00599	1.000	0.000	1a	1
14 C	C14	0.08068	0.24614	0.00531	1.000	0.000	1a	1
15 C	C15	0.10000	0.18119	0.04733	1.000	0.000	1a	1
16 C	C16	0.33025	0.07008	0.00632	1.000	0.000	1a	1
17 C	C17	0.41777	0.09651	0.04799	1.000	0.000	1a	1
18 C	C18	0.16559	0.10451	0.04755	1.000	0.000	1a	1
19 C	C19	0.64638	0.22480	0.00557	1.000	0.000	1a	1
20 C	C20	0.56033	0.16500	0.04766	1.000	0.000	1a	1
21 C	C21	0.91565	0.64358	0.00532	1.000	0.000	1a	1
22 C	C22	0.75669	0.33017	0.00542	1.000	0.000	1a	1
23 C	C23	0.82028	0.41504	0.04741	1.000	0.000	1a	1
24 C	C24	0.89312	0.55796	0.04723	1.000	0.000	1a	1

25 C	C25	0.91460	0.76050	0.09470	1.000	0.000	1a	1
26 C	C26	0.89656	0.81251	0.14235	1.000	0.000	1a	1
27 C	C27	0.77820	0.91003	0.09526	1.000	0.000	1a	1
28 C	C28	0.82707	0.88648	0.14259	1.000	0.000	1a	1
29 C	C29	0.36661	0.77896	0.09514	1.000	0.000	1a	1
30 C	C30	0.65359	0.91348	0.09549	1.000	0.000	1a	1
31 C	C31	0.58204	0.89132	0.14292	1.000	0.000	1a	1
32 C	C32	0.23798	0.65557	0.09501	1.000	0.000	1a	1
33 C	C33	0.18931	0.58311	0.14241	1.000	0.000	1a	1
34 C	C34	0.43801	0.82490	0.14277	1.000	0.000	1a	1
35 C	C35	0.09068	0.36801	0.09467	1.000	0.000	1a	1
36 C	C36	0.11565	0.43936	0.14233	1.000	0.000	1a	1
37 C	C37	0.22234	0.08993	0.09529	1.000	0.000	1a	1
38 C	C38	0.08564	0.23909	0.09476	1.000	0.000	1a	1
39 C	C39	0.10398	0.18735	0.14242	1.000	0.000	1a	1
40 C	C40	0.34698	0.08668	0.09550	1.000	0.000	1a	1
41 C	C41	0.41839	0.10831	0.14294	1.000	0.000	1a	1
42 C	C42	0.17352	0.11345	0.14262	1.000	0.000	1a	1
43 C	C43	0.63387	0.22079	0.09515	1.000	0.000	1a	1
44 C	C44	0.56240	0.17463	0.14277	1.000	0.000	1a	1
45 C	C45	0.90968	0.63157	0.09464	1.000	0.000	1a	1
46 C	C46	0.76255	0.34399	0.09502	1.000	0.000	1a	1
47 C	C47	0.81094	0.41644	0.14245	1.000	0.000	1a	1
48 C	C48	0.88448	0.56027	0.14233	1.000	0.000	1a	1
49 C	C49	0.91366	0.76029	0.18956	1.000	0.000	1a	1
50 C	C50	0.89420	0.81080	0.23691	1.000	0.000	1a	1

51 C	C51	0.77481	0.90425	0.18978	1.000	0.000	1a	1
52 C	C52	0.82417	0.88378	0.23699	1.000	0.000	1a	1
53 C	C53	0.36655	0.77446	0.18977	1.000	0.000	1a	1
54 C	C54	0.65147	0.90679	0.18989	1.000	0.000	1a	1
55 C	C55	0.58100	0.88816	0.23687	1.000	0.000	1a	1
56 C	C56	0.24045	0.65243	0.18968	1.000	0.000	1a	1
57 C	C57	0.19038	0.58165	0.23684	1.000	0.000	1a	1
58 C	C58	0.43738	0.82142	0.23693	1.000	0.000	1a	1
59 C	C59	0.09353	0.36791	0.18947	1.000	0.000	1a	1
60 C	C60	0.11633	0.43835	0.23676	1.000	0.000	1a	1
61 C	C61	0.22581	0.09576	0.18979	1.000	0.000	1a	1
62 C	C62	0.08695	0.23974	0.18957	1.000	0.000	1a	1
63 C	C63	0.10617	0.18912	0.23693	1.000	0.000	1a	1
64 C	C64	0.34896	0.09299	0.18991	1.000	0.000	1a	1
65 C	C65	0.41934	0.11119	0.23691	1.000	0.000	1a	1
66 C	C66	0.17629	0.11630	0.23698	1.000	0.000	1a	1
67 C	C67	0.63385	0.22457	0.18981	1.000	0.000	1a	1
68 C	C68	0.56301	0.17733	0.23698	1.000	0.000	1a	1
69 C	C69	0.90665	0.63184	0.18949	1.000	0.000	1a	1
70 C	C70	0.75977	0.34708	0.18971	1.000	0.000	1a	1
71 C	C71	0.80954	0.41811	0.23687	1.000	0.000	1a	1
72 C	C72	0.88366	0.56146	0.23677	1.000	0.000	1a	1
73 C	C73	0.90953	0.75838	0.28433	1.000	0.000	1a	1
74 C	C74	0.88737	0.80752	0.33126	1.000	0.000	1a	1
75 C	C75	0.77315	0.90439	0.28412	1.000	0.000	1a	1
76 C	C76	0.81905	0.88124	0.33126	1.000	0.000	1a	1

77 C	C77	0.36717	0.77262	0.28427	1.000	0.000	1a	1
78 C	C78	0.65004	0.90694	0.28418	1.000	0.000	1a	1
79 C	C79	0.57985	0.88737	0.33126	1.000	0.000	1a	1
80 C	C80	0.24123	0.65058	0.28428	1.000	0.000	1a	1
81 C	C81	0.19248	0.57985	0.33126	1.000	0.000	1a	1
82 C	C82	0.43782	0.81905	0.33126	1.000	0.000	1a	1
83 C	C83	0.09488	0.36803	0.28415	1.000	0.000	1a	1
84 C	C84	0.11876	0.43782	0.33126	1.000	0.000	1a	1
85 C	C85	0.22693	0.09554	0.28409	1.000	0.000	1a	1
86 C	C86	0.09055	0.24144	0.28433	1.000	0.000	1a	1
87 C	C87	0.11263	0.19248	0.33126	1.000	0.000	1a	1
88 C	C88	0.35008	0.09292	0.28416	1.000	0.000	1a	1
89 C	C89	0.42015	0.11263	0.33126	1.000	0.000	1a	1
90 C	C90	0.18095	0.11876	0.33126	1.000	0.000	1a	1
91 C	C91	0.63307	0.22674	0.28429	1.000	0.000	1a	1
92 C	C92	0.56218	0.18095	0.33126	1.000	0.000	1a	1
93 C	C93	0.90522	0.63195	0.28415	1.000	0.000	1a	1
94 C	C94	0.75873	0.34926	0.28432	1.000	0.000	1a	1
95 C	C95	0.80752	0.42015	0.33126	1.000	0.000	1a	1
96 C	C96	0.88124	0.56218	0.33126	1.000	0.000	1a	1
97 C	C97	0.90431	0.75601	0.37858	1.000	0.000	1a	1
98 C	C98	0.88737	0.80752	0.42590	1.000	0.000	1a	1
99 C	C99	0.76975	0.90120	0.37858	1.000	0.000	1a	1
100 C	C100	0.81905	0.88124	0.42590	1.000	0.000	1a	1
101 C	C101	0.36855	0.76975	0.37858	1.000	0.000	1a	1
102 C	C102	0.64830	0.90431	0.37858	1.000	0.000	1a	1

103 C	C103	0.57985	0.88737	0.42590	1.000	0.000	1a	1
104 C	C104	0.24399	0.64830	0.37858	1.000	0.000	1a	1
105 C	C105	0.19248	0.57985	0.42590	1.000	0.000	1a	1
106 C	C106	0.43782	0.81905	0.42590	1.000	0.000	1a	1
107 C	C107	0.09880	0.36855	0.37858	1.000	0.000	1a	1
108 C	C108	0.11876	0.43782	0.42590	1.000	0.000	1a	1
109 C	C109	0.23025	0.09880	0.37858	1.000	0.000	1a	1
110 C	C110	0.09569	0.24399	0.37858	1.000	0.000	1a	1
111 C	C111	0.11263	0.19248	0.42590	1.000	0.000	1a	1
112 C	C112	0.35170	0.09569	0.37858	1.000	0.000	1a	1
113 C	C113	0.42015	0.11263	0.42590	1.000	0.000	1a	1
114 C	C114	0.18095	0.11876	0.42590	1.000	0.000	1a	1
115 C	C115	0.63145	0.23025	0.37858	1.000	0.000	1a	1
116 C	C116	0.56218	0.18095	0.42590	1.000	0.000	1a	1
117 C	C117	0.90120	0.63145	0.37858	1.000	0.000	1a	1
118 C	C118	0.75601	0.35170	0.37858	1.000	0.000	1a	1
119 C	C119	0.80752	0.42015	0.42590	1.000	0.000	1a	1
120 C	C120	0.88124	0.56218	0.42590	1.000	0.000	1a	1
121 C	C121	0.90431	0.75601	0.47322	1.000	0.000	1a	1
122 C	C122	0.88737	0.80752	0.52055	1.000	0.000	1a	1
123 N	N123	0.76975	0.90120	0.47322	1.000	0.000	1a	1
124 C	C124	0.81905	0.88124	0.52055	1.000	0.000	1a	1
125 C	C125	0.36855	0.76975	0.47322	1.000	0.000	1a	1
126 C	C126	0.64830	0.90431	0.47322	1.000	0.000	1a	1
127 C	C127	0.57985	0.88737	0.52055	1.000	0.000	1a	1
128 C	C128	0.24399	0.64830	0.47322	1.000	0.000	1a	1

129 C	C129	0.19248	0.57985	0.52055	1.000	0.000	1a	1
130 N	N130	0.43782	0.81905	0.52055	1.000	0.000	1a	1
131 C	C131	0.09880	0.36855	0.47322	1.000	0.000	1a	1
132 C	C132	0.11876	0.43782	0.52055	1.000	0.000	1a	1
133 C	C133	0.23025	0.09880	0.47322	1.000	0.000	1a	1
134 C	C134	0.09569	0.24399	0.47322	1.000	0.000	1a	1
135 N	N135	0.11263	0.19248	0.52055	1.000	0.000	1a	1
136 C	C136	0.35170	0.09569	0.47322	1.000	0.000	1a	1
137 C	C137	0.42015	0.11263	0.52055	1.000	0.000	1a	1
138 C	C138	0.18095	0.11876	0.52055	1.000	0.000	1a	1
139 C	C139	0.63145	0.23025	0.47322	1.000	0.000	1a	1
140 N	N140	0.56218	0.18095	0.52055	1.000	0.000	1a	1
141 C	C141	0.90120	0.63145	0.47322	1.000	0.000	1a	1
142 C	C142	0.75601	0.35170	0.47322	1.000	0.000	1a	1
143 C	C143	0.80752	0.42015	0.52055	1.000	0.000	1a	1
144 C	C144	0.88124	0.56218	0.52055	1.000	0.000	1a	1
145 C	C145	0.90431	0.75601	0.56787	1.000	0.000	1a	1
146 C	C146	0.88737	0.80752	0.61519	1.000	0.000	1a	1
147 C	C147	0.76975	0.90120	0.56787	1.000	0.000	1a	1
148 C	C148	0.81905	0.88124	0.61519	1.000	0.000	1a	1
149 C	C149	0.36855	0.76975	0.56787	1.000	0.000	1a	1
150 C	C150	0.64830	0.90431	0.56787	1.000	0.000	1a	1
151 C	C151	0.57985	0.88737	0.61519	1.000	0.000	1a	1
152 C	C152	0.24399	0.64830	0.56787	1.000	0.000	1a	1
153 C	C153	0.19248	0.57985	0.61519	1.000	0.000	1a	1
154 C	C154	0.43782	0.81905	0.61519	1.000	0.000	1a	1

155	C	C155	0.09880	0.36855	0.56787	1.000	0.000	1a	1
156	N	N156	0.11876	0.43782	0.61519	1.000	0.000	1a	1
157	C	C157	0.23025	0.09880	0.56787	1.000	0.000	1a	1
158	C	C158	0.09569	0.24399	0.56787	1.000	0.000	1a	1
159	C	C159	0.11263	0.19248	0.61519	1.000	0.000	1a	1
160	N	N160	0.35170	0.09569	0.56787	1.000	0.000	1a	1
161	C	C161	0.42015	0.11263	0.61519	1.000	0.000	1a	1
162	C	C162	0.18095	0.11876	0.61519	1.000	0.000	1a	1
163	C	C163	0.63145	0.23025	0.56787	1.000	0.000	1a	1
164	C	C164	0.56218	0.18095	0.61519	1.000	0.000	1a	1
165	N	N165	0.90120	0.63145	0.56787	1.000	0.000	1a	1
166	C	C166	0.75601	0.35170	0.56787	1.000	0.000	1a	1
167	C	C167	0.80752	0.42015	0.61519	1.000	0.000	1a	1
168	C	C168	0.88124	0.56218	0.61519	1.000	0.000	1a	1
169	Co	Co169	0.51837	0.49721	0.52594	1.000	0.000	1a	1
170	Co	Co170	0.51837	0.65019	0.59354	1.000	0.000	1a	1
171	Co	Co171	0.69501	0.58554	0.59354	1.000	0.000	1a	1
172	Co	Co172	0.69501	0.73852	0.52594	1.000	0.000	1a	1
173	Co	Co173	0.51837	0.34424	0.45835	1.000	0.000	1a	1
174	Co	Co174	0.34172	0.40889	0.45835	1.000	0.000	1a	1
175	Co	Co175	0.51837	0.65019	0.45835	1.000	0.000	1a	1
176	Co	Co176	0.69501	0.58554	0.45835	1.000	0.000	1a	1
177	Co	Co177	0.34172	0.25591	0.52594	1.000	0.000	1a	1
178	Co	Co178	0.51837	0.34424	0.59354	1.000	0.000	1a	1
179	Co	Co179	0.69501	0.43256	0.52594	1.000	0.000	1a	1
180	Co	Co180	0.34172	0.40889	0.59354	1.000	0.000	1a	1

181	Co	Co181	0.34172	0.56187	0.52594	1.000	0.000	1a	1

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