Supporting Information

Unusual N-oxido formation in the peroxidation of cobalt(II) ethylenediaminetetraacetates

Yu-Chen Yang,[a,b] Rui Wu,[b] Yan Cai[b] and Zhao-Hui Zhou*[b]

[a]*Shaanxi Key Laboratory of Natural Products & Chemical Biology, College of Science, Northwest A&F University, Yangling 712100, People's Republic of China.*

[b]*State Key Laboratory of Physical Chemistry of Solid Surfaces, College of Chemistry and Chemical Engineering, Xiamen University, Xiamen, 361005, People's Republic of China. E-mail: zhzhou@xmu.edu.cn; Tel: +86 592 2184531; Fax: +86 592 2183047.*

Figure S1

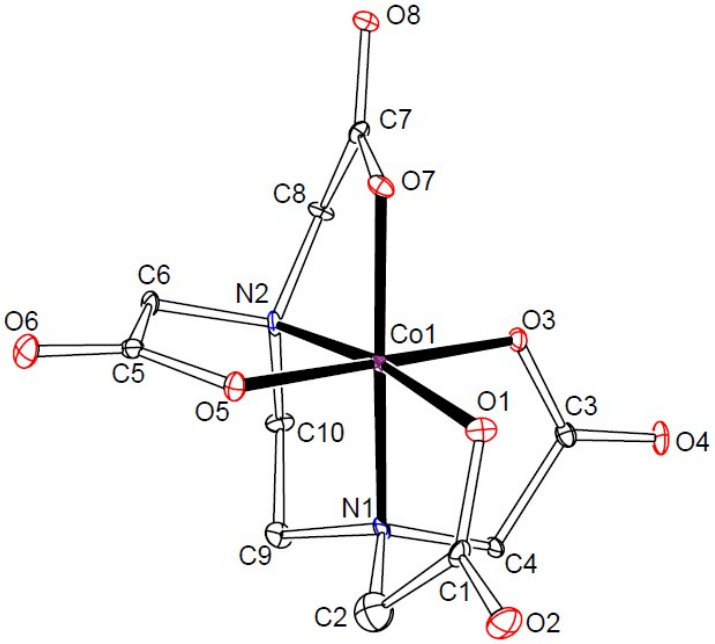

Figure S2

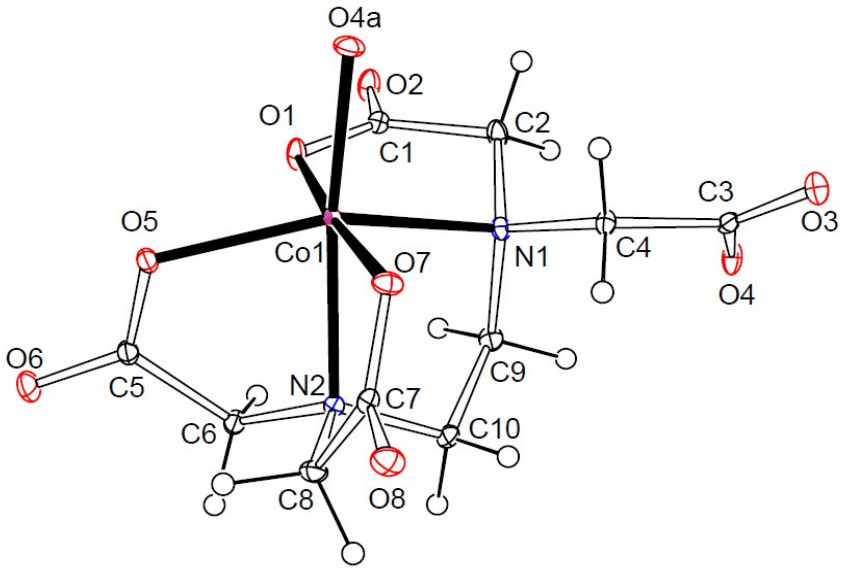

Figure S3

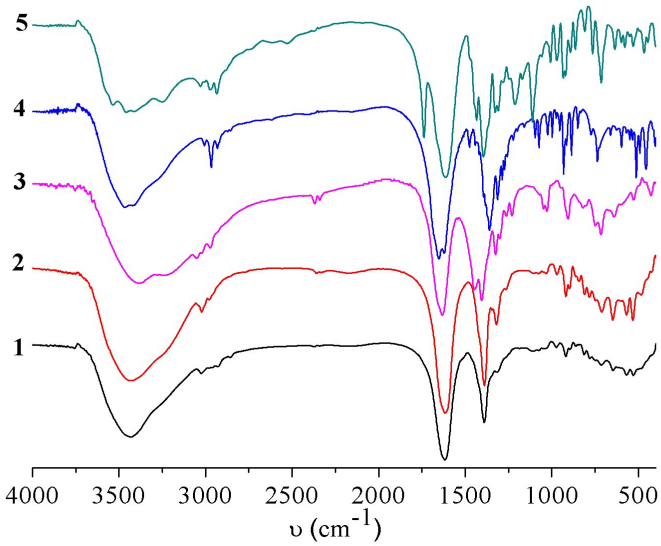

Figure S4

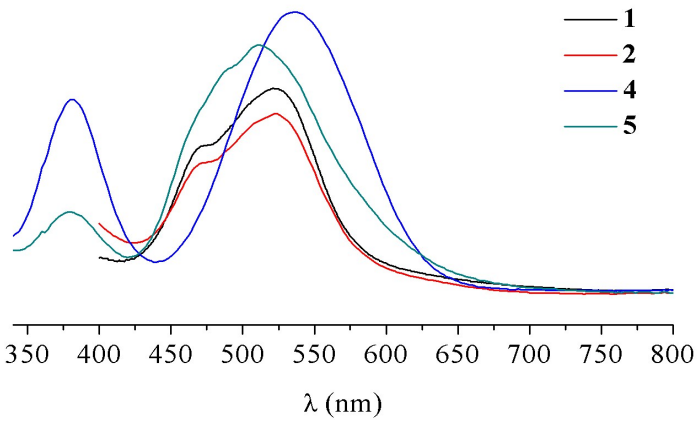

Table S1 Bond valence sum calculations for cobalt complexes **1** ~ **5**.

Co^{n+}	Complexes	Co1	Co2
+2	$K_4[Co_2(edtaO_2)_2]\cdot 6.5H_2O$ (**1**)	2.091	2.122
+2	$K_4[Co_2(edtaO_2)_2]\cdot 10H_2O$ (**2**)	2.179	2.112
+2	$[Co_2(edtaO_2)(H_2O)_6]_n\cdot 2nH_2O$(**3**)	2.146	
+3	$K[Co(edta)]\cdot 2H_2O$ (**4**)	3.778	
+2	$Na_{2n}[Co(edta)]_n\cdot 4nH_2O$ (**5**)	2.153	

Table S2. Selected bond distances for $K_4[Co_2(edtaO_2)_2]\cdot nH_2O$ [n = 6.5 (**1**), 10 (**2**)], $[Co_2(edtaO_2)(H_2O)_6]_n\cdot 2nH_2O$(**3**) and $\{Na_2[Co(edta)]\}_n\cdot 4nH_2O$ (**5**)

Bonds	**1**	**2**	Bonds	**3**	Bonds	**5**
Co(1)−O(1)	2.087(2)	2.097(3)	Co(1)-O(1)	2.078(1)	Co(1) −O(1)	2.140(2)
Co(1)−O(5)	2.144(2)	2.127(3)	Co(1)−O(3a)	2.111(1)	Co(1)−O(4)	2.033(2)
Co(1)−O(9)	2.040(2)	2.010(2)	Co(1)−O(5)	2.033(1)	Co(1)−O(5)	2.107(2)
Co(1)−O(10)	2.052(2)	2.070(2)	Co(1)−O(1w)	2.160(2)	Co(1)−O(7)	2.084(2)
Co(1)−O(11)	2.047(2)	2.107(2)	Co(1)− O(2w)	2.091(1)	Co(1)−N(1)	2.217(2)
Co(1)−O(19)	2.136(2)	2.070(2)	Co(1)− O(3w)	2.059(1)	Co(1)−N(2)	2.156(2)
Co(2)−O(7)	2.068(2)	2.081(2)				
Co(2)−O(10)	2.090(2)	2.056(2)				
Co(2)−O(13)	2.132(2)	2.138(3)				
Co(2)−O(17)	2.128(2)	2.088(3)				
Co(2)−O(19)	2.065(2)	2.067(2)				
Co(2)−O(20)	1.994(2)	1.987(2)				

Symmetry transformations: (a) $x - 1, y , z$.

Table S3. Selected bond distances and angles within the water clusters in $K_4[Co_2(edtaO_2)_2]\cdot 10H_2O$(**2**).

D–H···A	D–H (Å)	H···A(Å)	D···A(Å)	D–H···A(°)
O1w–H…O3w	0.85(3)	1.97(3)	2.802(4)	168(3)
O1w–H…O5wa	0.84(2)	1.99(2)	2.823(5)	167(4)
O3w–H…O10wb	0.85(3)	1.96(3)	2.789(5)	167(3)
O4w–H…O7wc	0.84(2)	2.10(1)	2.925(5)	167(4)
O5w–H…O4wa	0.85(2)	1.90(3)	2.719(5)	161(4)
O6w–H…O1wd	0.85(3)	2.07(3)	2.922(5)	177(2)
O8w–H…O9we	0.85(3)	1.98(3)	2.825(5)	174(3)
O9w–H…O7w	0.85(4)	2.20(4)	2.902(5)	140(3)
O10w–H…O1wc	0.85(3)	1.98(3)	2.794(5)	159(3)

Symmetry transformations: (a) $-x + 1, -y + 1, -z$; (b) $x, y + 1, z$; (c) $-x, -y, -z$; (d) $x + 1, y, z$; (e) $-x + 1, -y + 1, -z + 1$.

Table S4. ^{13}C NMR spectral data (in ppm) for K[Co(edta)]·$2H_2O$ (**4**) and K_4EDTA.

Compounds	$-CH_2N$	$-NCH_2CO_2$	$-CO_2$
4	66.1(12.4)	67.9(7.8), 68.1(8.0)	184.4(5.9), 185.1(6.6)
$[EDTA]^{4-}$	53.7	60.1	178.5