Supporting Information

A new hexanuclear Fe(III) nanocluster: Synthesis, structure, magnetic properties, and efficient activity as a precatalyst in water oxidation

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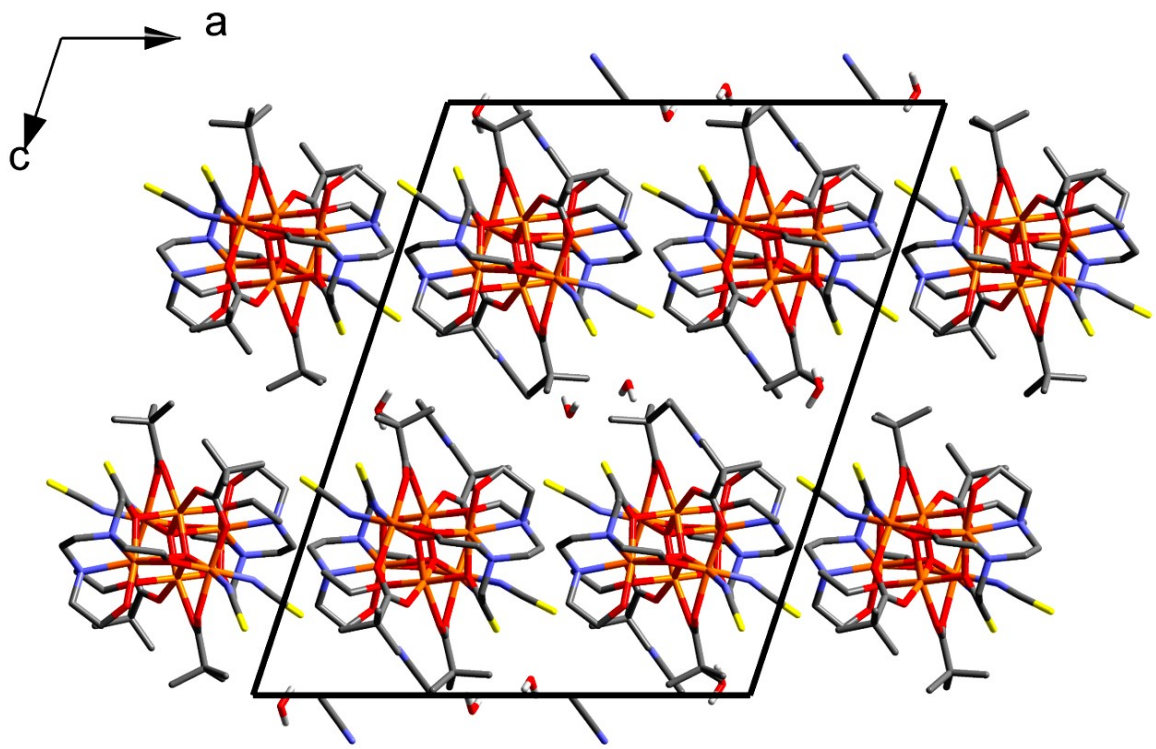

Figure S1. Packing view of the complex, **1.**

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

Empirical formula	$C_{48}H_{88}N_{10}O_{20}S_4Fe_6$
Formula weight	1588.62
Temperature/K	120(2)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	20.5565(10)
b/Å	13.6140(6)
c/Å	26.1065(14)
α/°	90
β/°	107.997(2)
γ/°	90
Volume/Å^3	6948.6(6)
Z	4
ρ_{calc}g/cm^3	1.519
μ/mm^{-1}	1.412
F(000)	3304.0
Crystal size/mm^3	0.093 × 0.072 × 0.066
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.396 to 50.998
Index ranges	$-24 \le h \le 24$, $-16 \le k \le 16$, $-31 \le l \le 31$
Reflections collected	92301
Independent reflections	12938 [R_{int} = 0.0840, R_{sigma} = 0.0480]
Data/restraints/parameters	12938/28/822
Goodness-of-fit on F^2	1.119
Final R indexes [I>=2σ (I)]	R_1 = 0.0564, wR_2 = 0.1270
Final R indexes [all data]	R_1 = 0.0865, wR_2 = 0.1399
Largest diff. peak/hole / e Å^{-3}	1.65/-0.93

$$R_1 = \sum \frac{||F_0| - |F_c||}{\sum |F_0|} \quad wR_2 = \left\{ \sum \frac{w(F_0^2 - F_c^2)^2}{\sum [wF_0^2]^2} \right\}^{\frac{1}{2}}$$

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Table S2. Bond lengths (Å) and bond angles (°) for **1**.

Fe1-O2	1.956(3)	Fe1-O1	1.996(3)
Fe1-O4	2.000(4)	Fe1-O6	2.023(3)
Fe1-O3	2.028(4)	Fe1-O5	2.041(3)
Fe1-Fe4	2.9392(10)	Fe2-O1	1.912(3)
Fe2-O17	1.982(4)	Fe2-N2	2.042(5)
Fe2-O7	2.060(4)	Fe2-O8	2.071(4)
Fe2-N1	2.087(5)	Fe3-O2	1.921(3)
Fe3-O10	1.982(4)	Fe3-N3	2.042(5)
Fe3-O11	2.056(4)	Fe3-O9	2.068(4)
Fe3-N4	2.072(5)	Fe4-O1	1.960(3)
Fe4-O2	1.988(4)	Fe4-O14	1.994(4)
Fe4-O15	2.021(4)	Fe4-O12	2.033(4)
Fe4-O13	2.045(3)	Fe5-O13	1.964(4)
Fe5-O10	1.980(4)	Fe5-O6	2.005(4)
Fe5-O16	2.118(4)	Fe5-N6	2.244(4)
Fe5-N5	2.270(4)	Fe5-O2	2.363(3)
Fe6-O5	1.963(4)	Fe6-O17	1.982(4)
Fe6-O12	1.992(4)	Fe6-O18	2.119(4)
Fe6-N7	2.249(4)	Fe6-N8	2.278(4)
Fe6-O1	2.362(3)		
Fe2-O1-Fe4	130.12(19)	Fe2-O1-Fe1	129.41(18)
Fe4-O1-Fe1	95.96(15)	Fe2-O1-Fe6	96.14(14)
Fe4-O1-Fe6	99.06(14)	Fe1-O1-Fe6	95.58(14)
Fe3-O2-Fe1	130.74(19)	Fe3-O2-Fe4	128.53(18)
Fe1-O2-Fe4	96.34(15)	Fe3-O2-Fe5	95.66(14)
Fe1-O2-Fe5	99.03(14)	Fe4-O2-Fe5	95.90(13)
Fe6-O5-Fe1	107.89(16)	C21-O6-Fe5	120.3(3)
Fe5-O13-Fe4	107.89(16)	C36-O14-Fe4	134.5(4)
Fe6-O17-Fe2	107.36(17)	C19-O18-Fe6	117.6(3)

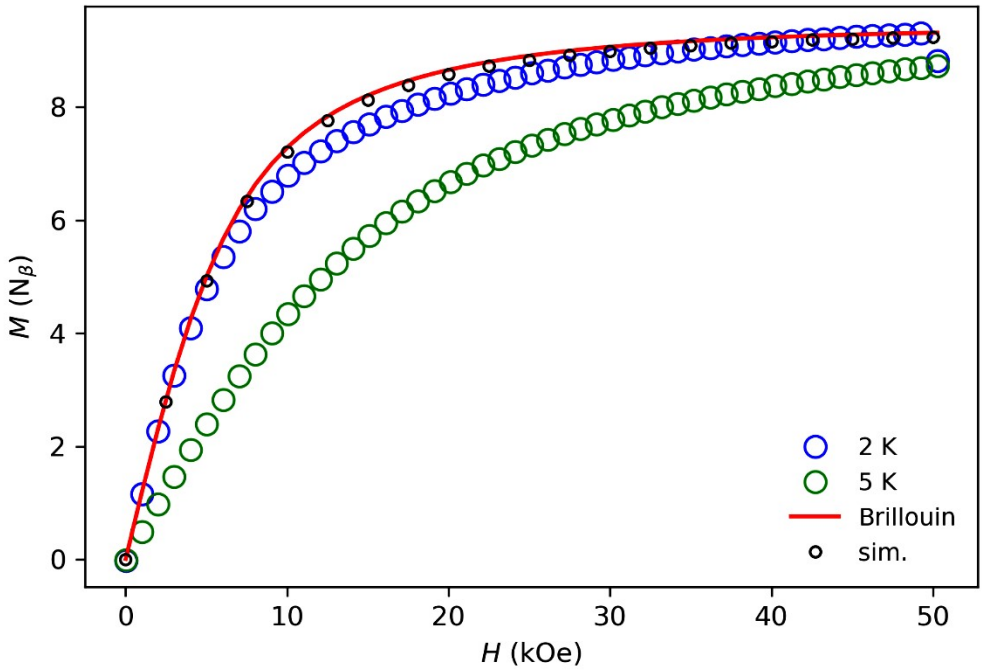

Figure S2. Field dependence of the magnetization for **1** at 2 (blue circles) and 5 K (green circles), red line is Brillouin function, the none filled style circle with black color is the simulated data by MagPack and the exchange model used and described in the text.

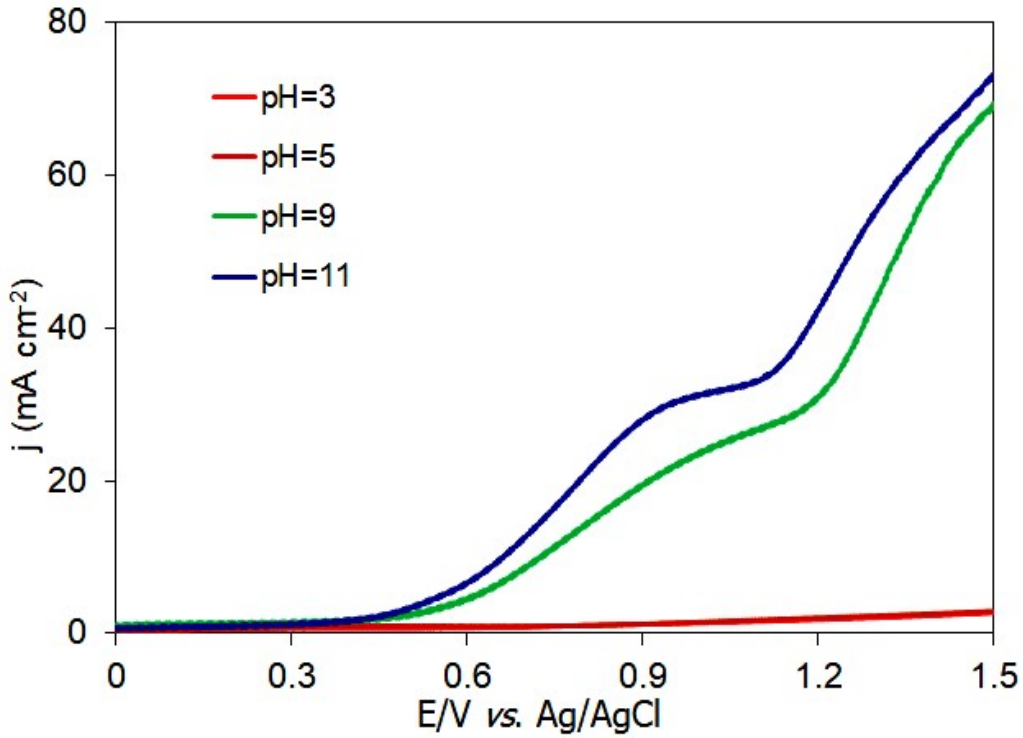

Figure S3. LSV curves of carbon paste electrode modified by **1** at different pH in a scan rate of 50 mV s^{-1}.

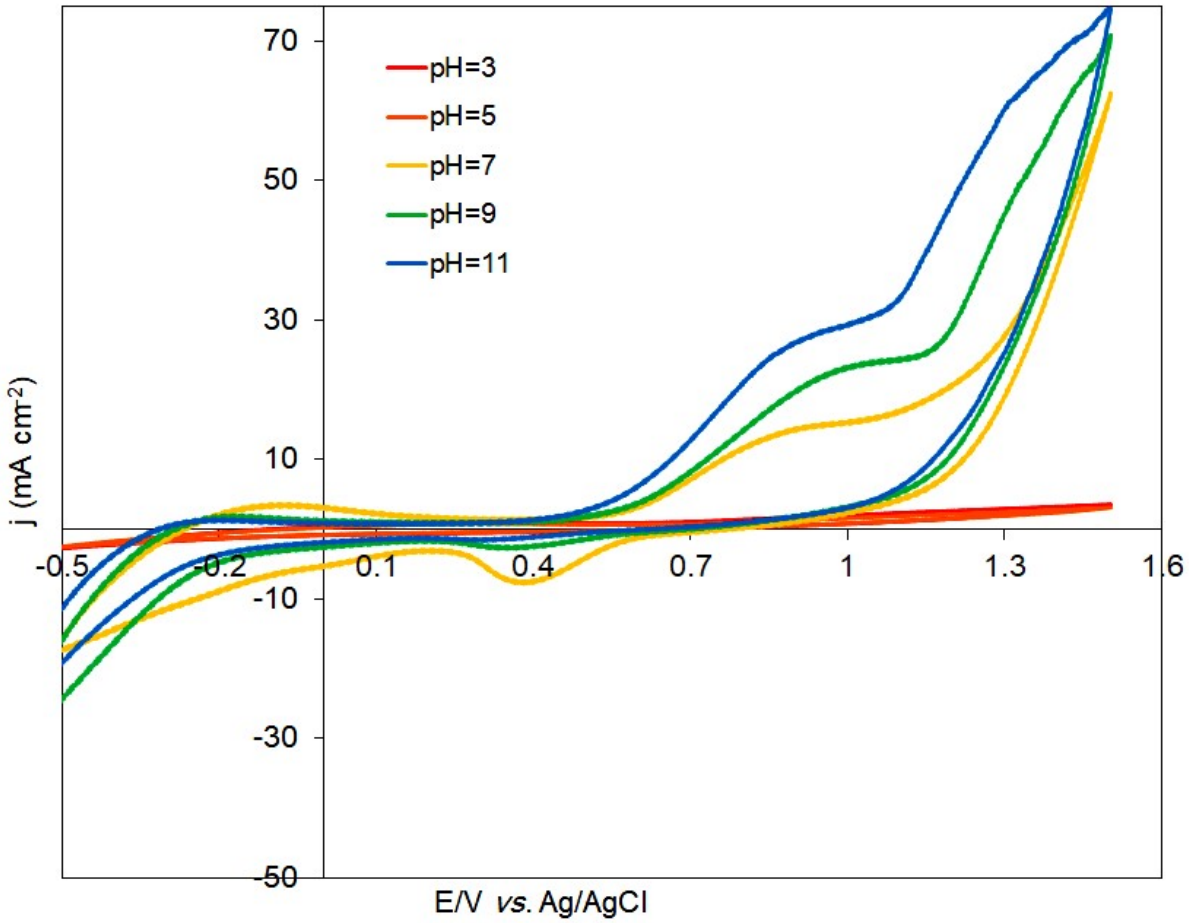

Figure S4. CV for carbon paste electrode modified by **1** at different pH in a scan rate of 50 mV s^{-1}.

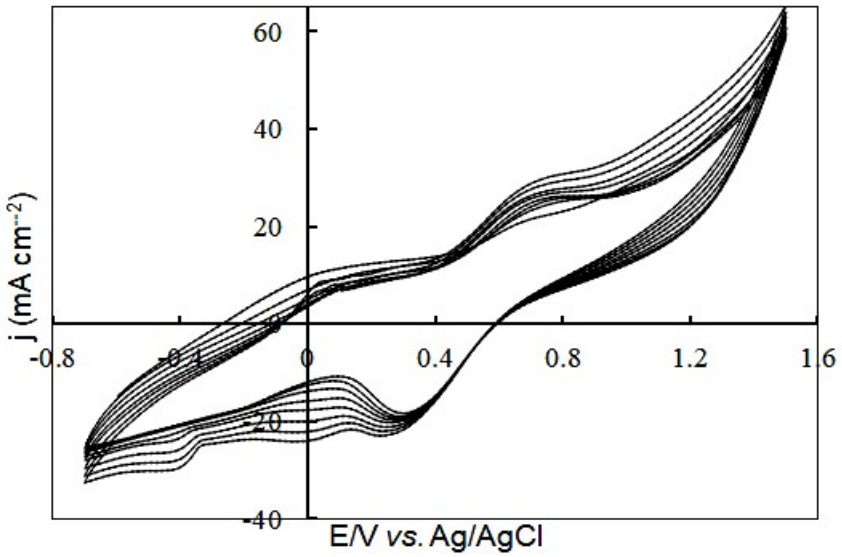

Figure S5. Continuous CVs (first ten cycles) for the carbon paste electrode modified by **1** in a borate solution (0.5 M) at pH = 7 and scan rate of 50 $mV.s^{-1}$ in the range of -0.7-1.5 V *vs.* Ag/AgCl.

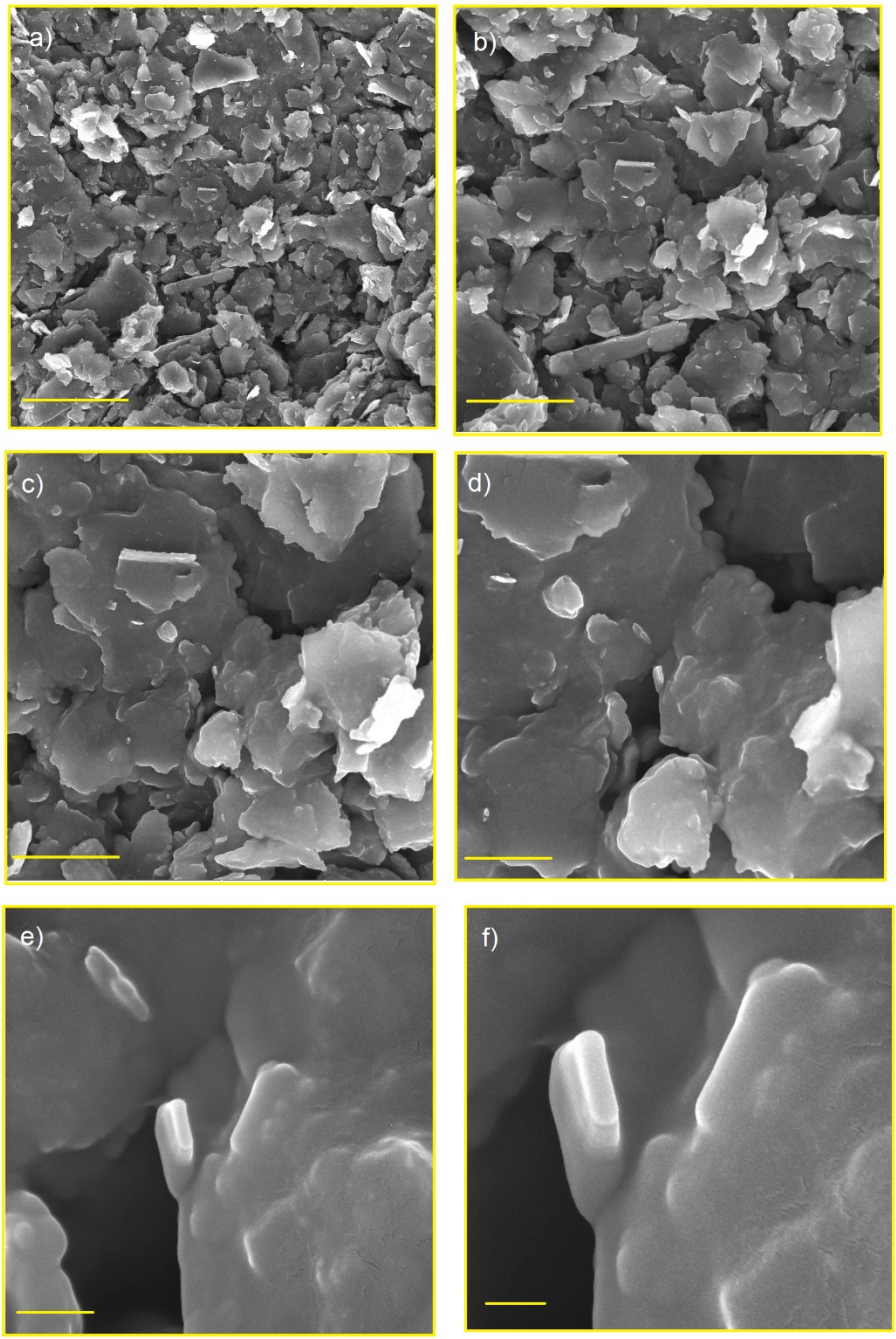

Figure S6. FE-SEM images of the electrode surface before water oxidation in different scales; 20 µm(a), 10 µm(b), 2 µm (c), 1 µM (d), 500 nm (e) and 200 nm (f).

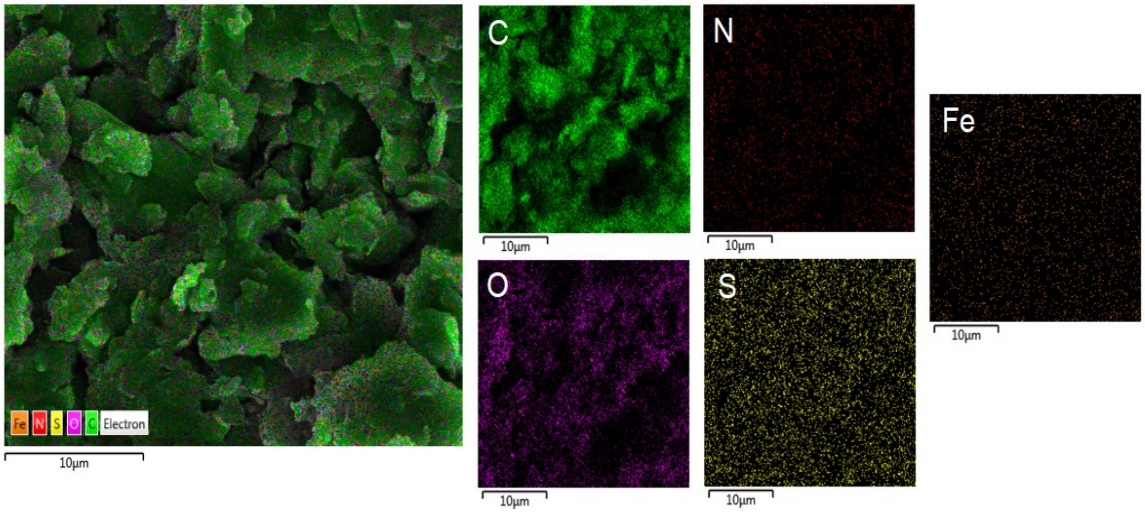

Figure S7. SEM/EDX images showing the elemental distribution of C, O, N, S, and Fe in the electrode surface before water oxidation

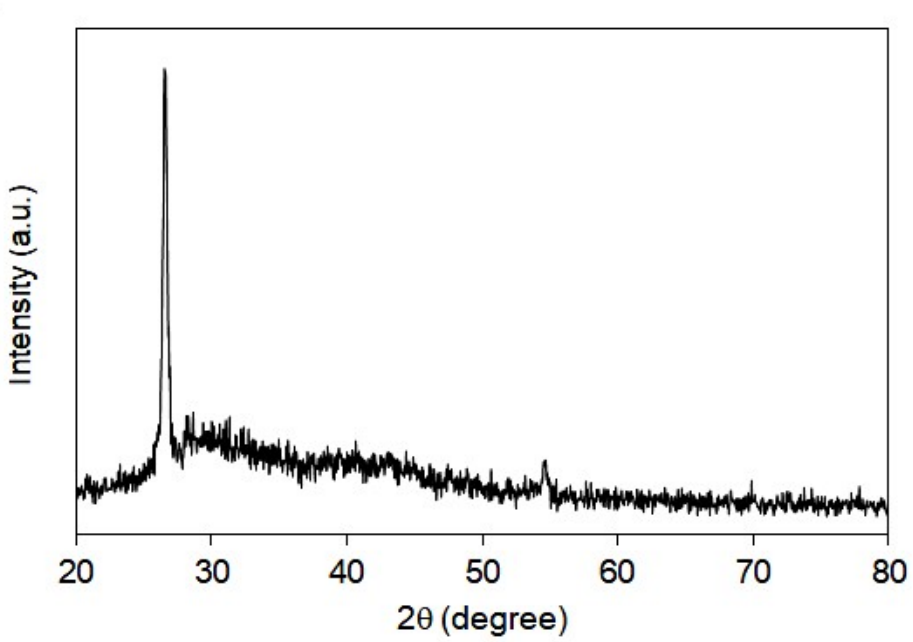

Figure S8. XRD pattern of the surface electrode before continuous CVs in 0.5 M of borate buffer at pH=7.

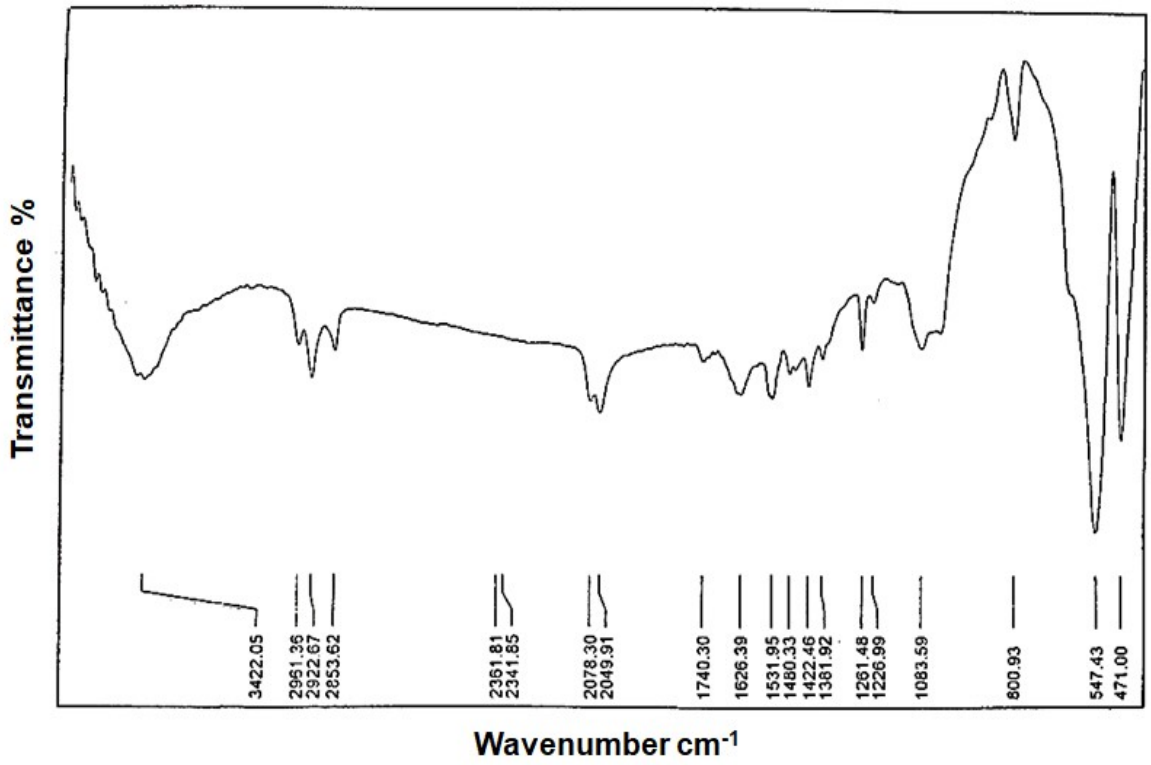

Figure S9: FT-IR spectra of the surface of the modified electrode with the Fe cluster after continuous CVs in a 0.5 M borate solution (pH=7) at the scan rate of 50 mV s^{-1}.

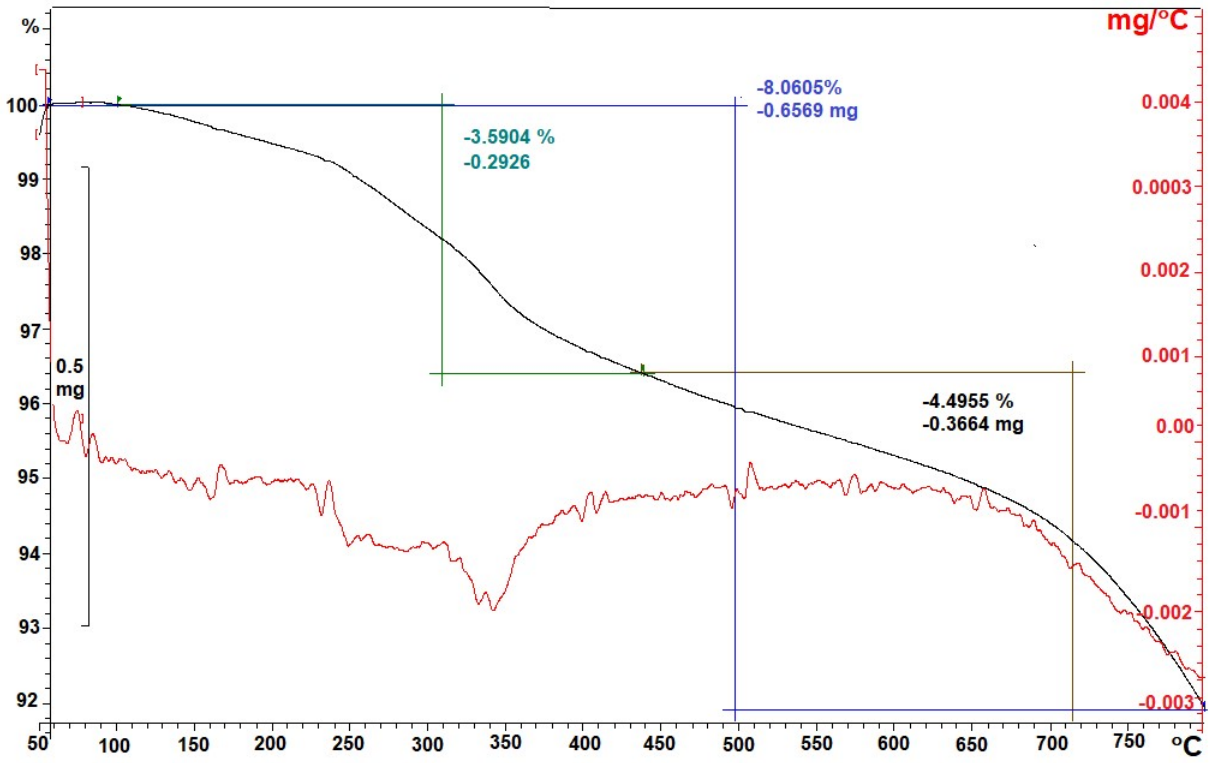

Figure S10: TGA plot of the surface of the modified electrode with the Fe cluster after continuous CVs in a 0.5 M borate solution (pH=7) at the scan rate of 50 mV s^{-1}.