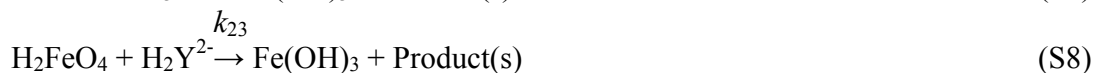
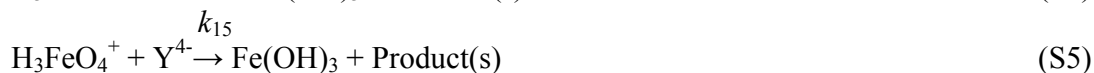
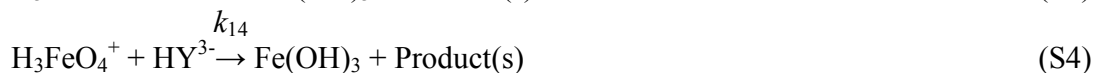
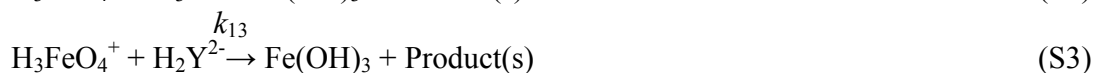
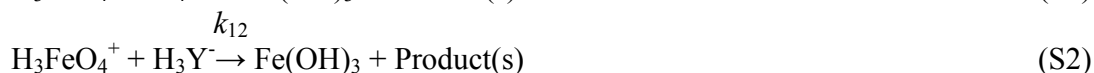


Text S1

In the pH range studied, all four species of Fe(VI) (H_3FeO_4^+ , H_2FeO_4 , HFeO_4^- , FeO_4^{2-}) can possibly react with the five species of EDTA (H_4Y , H_3Y^- , H_2Y^{2-} , HY^{3-} , and Y^{4-}) (equations S1-S20).



The rate of disappearance of Fe(VI) is given by:

$$\begin{aligned}
 -d[\text{Fe(VI)}]_{\text{tot}}/dt = & k_{11}[\text{H}_3\text{FeO}_4^+][\text{H}_4\text{Y}] + k_{12}[\text{H}_3\text{FeO}_4^+][\text{H}_3\text{Y}^-] + k_{13}[\text{H}_3\text{FeO}_4^+][\text{H}_2\text{Y}^{2-}] \\
 & k_{14}[\text{H}_3\text{FeO}_4^+][\text{HY}^{3-}] + k_{15}[\text{H}_3\text{FeO}_4^+][\text{Y}^{4-}] + k_{21}[\text{H}_2\text{FeO}_4][\text{H}_4\text{Y}] + k_{22}[\text{H}_2\text{FeO}_4][\text{H}_3\text{Y}^-] + \\
 & k_{23}[\text{H}_2\text{FeO}_4][\text{H}_2\text{Y}^{2-}] + k_{24}[\text{H}_2\text{FeO}_4][\text{HY}^{3-}] + k_{25}[\text{H}_2\text{FeO}_4][\text{Y}^{4-}] + k_{31}[\text{HFeO}_4^-][\text{H}_4\text{Y}] + k_{32}[\text{HFeO}_4^-] \\
 & [\text{H}_3\text{Y}^-] + k_{33}[\text{HFeO}_4^-][\text{H}_2\text{Y}^{2-}] + k_{34}[\text{HFeO}_4^-][\text{HY}^{3-}] + k_{35}[\text{HFeO}_4^-][\text{Y}^{4-}] + k_{41}[\text{FeO}_4^{2-}][\text{H}_4\text{Y}] + \\
 & k_{42}[\text{FeO}_4^{2-}][\text{H}_3\text{Y}^-] + k_{43}[\text{FeO}_4^{2-}][\text{H}_2\text{Y}^{2-}] + k_{44}[\text{FeO}_4^{2-}][\text{HY}^{3-}] + k_{45}[\text{FeO}_4^{2-}][\text{Y}^{4-}] \quad (\text{I})
 \end{aligned}$$

By using the fraction of speciation of Fe(VI) and glycine (K_{a1} , K_{a2} , and K_{a3} are the equilibrium constants involving H_3FeO_4^+ , H_2FeO_4 and HFeO_4^- ; K_3 , K_4 , K_5 , and K_6 are the equilibrium constants involving H_4EDTA , H_3EDTA^- , $\text{H}_2\text{EDTA}^{2-}$, and HEDTA^{3-}), equation I can then be written as:

$$\begin{aligned}
 -d[\text{Fe(VI)}]_{\text{tot}}/dt = & [(k_{11}[\text{H}^+]^7 + k_{12}K_3[\text{H}^+]^6 + k_{13}K_3K_4[\text{H}^+]^5 + k_{14}K_3K_4K_5[\text{H}^+]^4 + k_{15}K_3K_4K_5K_6[\text{H}^+]^3 + k_{21}K_{a1}[\text{H}^+]^6 + k_{22}K_{a1}K_{a3}[\text{H}^+]^5 \\
 & + k_{23}K_{a1}K_3K_4[\text{H}^+]^4 + k_{24}K_{a1}K_3K_4K_5[\text{H}^+]^3 + k_{25}K_{a1}K_3K_4K_5K_6[\text{H}^+]^2 + k_{31}K_{a1}K_{a2}[\text{H}^+]^5 + k_{32}K_{a1}K_{a2}K_3[\text{H}^+]^4 \\
 & + k_{33}K_{a1}K_{a2}K_3K_4[\text{H}^+]^3 + k_{34}K_{a1}K_{a2}K_3K_4K_5[\text{H}^+]^2 + k_{35}K_{a1}K_{a2}K_3K_4K_5K_6[\text{H}^+] + k_{41}K_{a1}K_{a2}K_{a3}[\text{H}^+]^4 \\
 & + k_{42}K_{a1}K_{a2}K_{a3}K_3[\text{H}^+]^3 + k_{43}K_{a1}K_{a2}K_{a3}K_3K_4[\text{H}^+]^2 + k_{44}K_{a1}K_{a2}K_{a3}K_3K_4K_5[\text{H}^+] + k_{45}K_{a1}K_{a2}K_{a3}K_3K_4K_5K_6)/Z][\text{Fe(VI)}]_{\text{tot}}[\text{EDTA}]_{\text{tot}} \quad (\text{II})
 \end{aligned}$$

$$\begin{aligned}
 \text{where } Z = & [\text{H}^+]^7 + K_3[\text{H}^+]^6 + K_3K_4[\text{H}^+]^5 + K_3K_4K_5[\text{H}^+]^4 + K_3K_4K_5K_6[\text{H}^+]^3 + K_{a1}[\text{H}^+]^6 + \\
 & K_{a1}K_3[\text{H}^+]^5 + K_{a1}K_3K_4[\text{H}^+]^4 + K_{a1}K_3K_4K_5[\text{H}^+]^3 + K_{a1}K_3K_4K_5K_6[\text{H}^+]^2 + K_{a1}K_{a2}[\text{H}^+]^5 + \\
 & K_{a1}K_{a2}K_3[\text{H}^+]^4 + K_{a1}K_{a2}K_3K_4[\text{H}^+]^3 + K_{a1}K_{a2}K_3K_4K_5[\text{H}^+]^2 + K_{a1}K_{a2}K_3K_4K_5K_6[\text{H}^+] + \\
 & K_{a1}K_{a2}K_{a3}[\text{H}^+]^4 + K_{a1}K_{a2}K_{a3}K_3[\text{H}^+]^3 + K_{a1}K_{a2}K_{a3}K_3K_4[\text{H}^+]^2 + K_{a1}K_{a2}K_{a3}K_3K_4K_5[\text{H}^+] + \\
 & K_{a1}K_{a2}K_{a3}K_3K_4K_5K_6 \quad (\text{III})
 \end{aligned}$$

Table S1. Fe(VI) oxidation of EDTA at different pH at 25°C.

pH	[EDTA], M	k , $M^{-1}s^{-1}$	order(n)
1.98	$[0.25-1.00] \times 10^{-3}$	$(4.19 \pm 0.58) \times 10^4$	1.01 ± 0.13
2.16	$[0.25-1.00] \times 10^{-3}$	$(3.36 \pm 0.23) \times 10^4$	0.88 ± 0.08
2.42	$[0.60-1.50] \times 10^{-3}$	$(2.31 \pm 0.24) \times 10^4$	1.07 ± 0.12
2.72	$[0.60-1.50] \times 10^{-3}$	$(1.14 \pm 0.07) \times 10^4$	0.80 ± 0.03
3.43	$[1.20-1.50] \times 10^{-3}$	$(8.76 \pm 0.80) \times 10^3$	0.74 ± 0.04
3.46	$[0.13-1.00] \times 10^{-3}$	$(6.66 \pm 0.24) \times 10^3$	1.07 ± 0.05
3.79	$[1.20-1.50] \times 10^{-3}$	$(3.00 \pm 0.47) \times 10^3$	0.90 ± 0.05
3.87	$[0.50-2.00] \times 10^{-3}$	$(3.99 \pm 0.56) \times 10^3$	1.13 ± 0.11
4.04	$[0.75-1.00] \times 10^{-3}$	$(3.47 \pm 0.14) \times 10^3$	0.70 ± 0.04
4.18	$[0.75-1.00] \times 10^{-3}$	$(2.06 \pm 0.54) \times 10^3$	1.01 ± 0.11
4.29	$[1.20-1.50] \times 10^{-3}$	$(1.40 \pm 0.24) \times 10^3$	1.01 ± 0.11
4.30	$[1.50-2.00] \times 10^{-3}$	$(1.05 \pm 0.14) \times 10^3$	1.01 ± 0.11
4.56	$[1.20-1.50] \times 10^{-3}$	$(9.50 \pm 3.47) \times 10^2$	1.01 ± 0.11
4.76	$[0.75-1.00] \times 10^{-3}$	$(8.48 \pm 1.91) \times 10^2$	1.17 ± 0.12
4.80	$[1.20-1.50] \times 10^{-3}$	$(6.68 \pm 0.97) \times 10^2$	1.01 ± 0.11
4.96	$[0.75-1.00] \times 10^{-3}$	$(3.58 \pm 0.10) \times 10^2$	0.88 ± 0.10
5.22	$[0.75-1.00] \times 10^{-3}$	$(2.33 \pm 0.10) \times 10^2$	0.78 ± 0.08
5.30	$[0.25-1.00] \times 10^{-3}$	$(1.85 \pm 0.11) \times 10^2$	1.33 ± 0.14
5.46	$[0.50-1.00] \times 10^{-3}$	$(1.67 \pm 0.11) \times 10^2$	1.23 ± 0.12
5.82	$[0.50-1.00] \times 10^{-3}$	$(1.31 \pm 0.10) \times 10^2$	1.14 ± 0.11
6.07	$[0.50-1.00] \times 10^{-3}$	$(1.17 \pm 0.14) \times 10^2$	1.05 ± 0.10
6.50	$[1.00-1.25] \times 10^{-1}$	$(1.05 \pm 0.07) \times 10^2$	0.94 ± 0.10
7.00	$[1.00-1.25] \times 10^{-1}$	$(7.90 \pm 0.50) \times 10^1$	0.85 ± 0.09
7.50	$[1.35-1.50] \times 10^{-1}$	$(3.00 \pm 0.30) \times 10^1$	1.11 ± 0.12
8.00	$[1.00-1.25] \times 10^{-1}$	$(1.20 \pm 0.20) \times 10^1$	1.03 ± 0.11
8.50	$[0.30-1.25] \times 10^{-1}$	$(4.00 \pm 0.11) \times 10^0$	1.08 ± 0.01
9.00	$[0.05-1.00] \times 10^{-1}$	$(1.72 \pm 0.08) \times 10^0$	1.08 ± 0.02
9.24	$[0.30-2.00] \times 10^{-1}$	$(1.55 \pm 0.03) \times 10^0$	1.19 ± 0.01
9.45	$[0.30-1.50] \times 10^{-1}$	$(6.83 \pm 0.37) \times 10^{-1}$	1.13 ± 0.05
10.00	$[0.30-1.50] \times 10^{-1}$	$(6.00 \pm 0.40) \times 10^{-1}$	1.09 ± 0.05
10.14	$[0.30-1.50] \times 10^{-1}$	$(3.66 \pm 0.14) \times 10^{-1}$	1.09 ± 0.04
10.50	$[0.30-1.50] \times 10^{-1}$	$(3.30 \pm 0.20) \times 10^{-1}$	1.11 ± 0.04
10.68	$[0.30-1.50] \times 10^{-1}$	$(2.76 \pm 0.28) \times 10^{-1}$	1.03 ± 0.16
11.00	$[0.40-1.00] \times 10^{-1}$	$(1.70 \pm 0.20) \times 10^{-1}$	1.19 ± 0.11
11.50	$[0.95-2.00] \times 10^{-1}$	$(1.08 \pm 0.08) \times 10^{-1}$	1.20 ± 0.12
12.00	$[0.95-2.00] \times 10^{-1}$	$(9.00 \pm 0.70) \times 10^{-2}$	0.93 ± 0.10
12.40	$[1.00-2.00] \times 10^{-1}$	$(8.60 \pm 0.80) \times 10^{-2}$	1.26 ± 0.14

Table S2. Rate constants for Fe(VI) oxidation of EDTA at different pH and temperatures.

Temp, K	pH=5.4 ¹	pH=7.1 ¹	pH=9.2 ¹
	$k, 10^2 \text{ M}^{-1}\text{s}^{-1}$	$k, 10^1 \text{ M}^{-1}\text{s}^{-1}$	$k, 10^0 \text{ M}^{-1}\text{s}^{-1}$
288	2.32±0.30	0.80±0.01	1.02±0.03
293	2.55±0.04	0.93±0.04	1.73±0.09
298	3.55±0.05	1.27±0.08	1.60±0.02
303	3.97±0.13	1.55±0.01	2.85±0.17
308	4.52±0.12	1.83±0.02	4.33±0.22
313	5.15±0.40	2.05±0.07	6.18±0.45
318	6.28±0.65	2.57±0.04	8.03±0.34

¹[EDTA]=0.5-1.0 x 10⁻³ M