Electronic Supplementary Information for Dalton Transactions

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).

$$H_3FeO_4^+ + H_4Y \xrightarrow{k_{11}} Fe(OH)_3 + \text{Product(s)} \quad (S1)$$

$$H_3FeO_4^+ + H_3Y^- \xrightarrow{k_{12}} Fe(OH)_3 + \text{Product(s)} \quad (S2)$$

$$H_3FeO_4^+ + H_2Y^{2-} \xrightarrow{k_{13}} Fe(OH)_3 + \text{Product(s)} \quad (S3)$$

$$H_3FeO_4^+ + HY^{3-} \xrightarrow{k_{14}} Fe(OH)_3 + \text{Product(s)} \quad (S4)$$

$$H_3FeO_4^+ + Y^{4-} \xrightarrow{k_{15}} Fe(OH)_3 + \text{Product(s)} \quad (S5)$$

$$H_2FeO_4 + H_4Y \xrightarrow{k_{21}} Fe(OH)_3 + \text{Product(s)} \quad (S6)$$

$$H_2FeO_4 + H_3Y^- \xrightarrow{k_{22}} Fe(OH)_3 + \text{Product(s)} \quad (S7)$$

$$H_2FeO_4 + H_2Y^{2-} \xrightarrow{k_{23}} Fe(OH)_3 + \text{Product(s)} \quad (S8)$$

$$H_2FeO_4 + HY^{3-} \xrightarrow{k_{24}} Fe(OH)_3 + \text{Product(s)} \quad (S9)$$

$$H_2FeO_4 + Y^{4-} \xrightarrow{k_{25}} Fe(OH)_3 + \text{Product(s)} \quad (S10)$$

$$HFeO_4^- + H_4Y \xrightarrow{k_{31}} Fe(OH)_3 + \text{Product(s)} \quad (S11)$$

$$HFeO_4^- + H_3Y^- \xrightarrow{k_{32}} Fe(OH)_3 + \text{Product(s)} \quad (S12)$$

$$HFeO_4^- + H_2Y^{2-} \xrightarrow{k_{33}} Fe(OH)_3 + \text{Product(s)} \quad (S13)$$

$$HFeO_4^- + HY^{3-} \xrightarrow{k_{34}} Fe(OH)_3 + \text{Product(s)} \quad (S14)$$

$$HFeO_4^- + Y^{4-} \xrightarrow{k_{35}} Fe(OH)_3 + \text{Product(s)} \quad (S15)$$

$$FeO_4^{2-} + H_4Y \xrightarrow{k_{41}} Fe(OH)_3 + \text{Product(s)} \quad (S16)$$

$$FeO_4^{2-} + H_3Y^- \xrightarrow{k_{42}} Fe(OH)_3 + \text{Product(s)} \quad (S17)$$

$$FeO_4^{2-} + H_2Y^{2-} \xrightarrow{k_{43}} Fe(OH)_3 + \text{Product(s)} \quad (S18)$$

$$FeO_4^{2-} + HY^{3-} \xrightarrow{k_{44}} Fe(OH)_3 + \text{Product(s)} \quad (S19)$$

$$FeO_4^{2-} + Y^{4-} \xrightarrow{k_{45}} Fe(OH)_3 + \text{Product(s)} \quad (S20)$$

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

$-d[Fe(VI)]_{tot}/dt = k_{11}[H_3FeO_4^+][H_4Y] + k_{12}[H_3FeO_4^+][H_3Y^-] + k_{13}[H_3FeO_4^+][H_2Y^{2-}]$ $k_{14}[H_3FeO_4^+][HY^{3-}] + k_{15}[H_3FeO_4^+][Y^{4-}] + k_{21}[H_2FeO_4][H_4Y] + k_{22}[H_2FeO_4][H_3Y^-] + k_{23}[H_2FeO_4][H_2Y^{2-}] + k_{24}[H_2FeO_4][HY^{3-}] + k_{25}[H_2FeO_4][Y^{4-}] + k_{31}[HFeO_4^-][H_4Y] + k_{32}[HFeO_4^-][H_3Y^-] + k_{33}[HFeO_4^-][H_2Y^{2-}] + k_{34}[HFeO_4^-][HY^{3-}] + k_{35}[HFeO_4^-][Y^{4-}] + k_{41}[FeO_4^{2-}][H_4Y] + k_{42}[FeO_4^{2-}][H_3Y^-] + k_{43}[FeO_4^{2-}][H_2Y^{2-}] + k_{44}[FeO_4^{2-}][HY^{3-}] + k_{45}[FeO_4^{2-}][Y^{4-}]$ (I)

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 and $HFeO_4^-$; K_3, K_4, K_5, and K_6 are the equilibrium constants involving H_4EDTA, H_3EDTA^-, H_2EDTA^{2-}, and $HEDTA^{3-}$), equation I can then be written as:

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

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

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] x 10^{-3}	(4.19±0.58) x 10^{4}	1.01±0.13
2.16	[0.25-1.00] x 10^{-3}	(3.36±0.23) x 10^{4}	0.88±0.08
2.42	[0.60-1.50] x 10^{-3}	(2.31±0.24) x 10^{4}	1.07±0.12
2.72	[0.60-1.50] x 10^{-3}	(1.14±0.07) x 10^{4}	0.80±0.03
3.43	[1.20-1.50] x 10^{-3}	(8.76±0.80) x 10^{3}	0.74±0.04
3.46	[0.13-1.00] x 10^{-3}	(6.66±0.24) x 10^{3}	1.07±0.05
3.79	[1.20-1.50] x 10^{-3}	(3.00±0.47) x 10^{3}	0.90±0.05
3.87	[0.50-2.00] x 10^{-3}	(3.99±0.56) x 10^{3}	1.13±0.11
4.04	[0.75-1.00] x 10^{-3}	(3.47±0.14) x 10^{3}	0.70±0.04
4.18	[0.75-1.00] x 10^{-3}	(2.06±0.54) x 10^{3}	1.01±0.11
4.29	[1.20-1.50] x 10^{-3}	(1.40±0.24) x 10^{3}	1.01±0.11
4.30	[1.50-2.00] x 10^{-3}	(1.05±0.14) x 10^{3}	1.01±0.11
4.56	[1.20-1.50] x 10^{-3}	(9.50±3.47) x 10^{2}	1.01±0.11
4.76	[0.75-1.00] x 10^{-3}	(8.48±1.91) x 10^{2}	1.17±0.12
4.80	[1.20-1.50] x 10^{-3}	(6.68±0.97) x 10^{2}	1.01±0.11
4.96	[0.75-1.00] x 10^{-3}	(3.58±0.10) x 10^{2}	0.88±0.10
5.22	[0.75-1.00] x 10^{-3}	(2.33±0.10) x 10^{2}	0.78±0.08
5.30	[0.25-1.00] x 10^{-3}	(1.85±0.11) x 10^{2}	1.33±0.14
5.46	[0.50-1.00] x 10^{-3}	(1.67±0.11) x 10^{2}	1.23±0.12
5.82	[0.50-1.00] x 10^{-3}	(1.31±0.10) x 10^{2}	1.14±0.11
6.07	[0.50-1.00] x 10^{-3}	(1.17±0.14) x 10^{2}	1.05±0.10
6.50	[1.00-1.25] x 10^{-1}	(1.05±0.07) x 10^{2}	0.94±0.10
7.00	[1.00-1.25] x 10^{-1}	(7.90±0.50) x 10^{1}	0.85±0.09
7.50	[1.35-1.50] x 10^{-1}	(3.00±0.30) x 10^{1}	1.11±0.12
8.00	[1.00-1.25] x 10^{-1}	(1.20±0.20) x 10^{1}	1.03±0.11
8.50	[0.30-1.25] x 10^{-1}	(4.00±0.11) x 10^{0}	1.08±0.01
9.00	[0.05-1.00] x 10^{-1}	(1.72±0.08) x 10^{0}	1.08±0.02
9.24	[0.30-2.00] x 10^{-1}	(1.55±0.03) x 10^{0}	1.19±0.01
9.45	[0.30-1.50] x 10^{-1}	(6.83±0.37) x 10^{-1}	1.13±0.05
10.00	[0.30-1.50] x 10^{-1}	(6.00±0.40) x 10^{-1}	1.09±0.05
10.14	[0.30-1.50] x 10^{-1}	(3.66±0.14) x 10^{-1}	1.09±0.04
10.50	[0.30-1.50] x 10^{-1}	(3.30±0.20) x 10^{-1}	1.11±0.04
10.68	[0.30-1.50] x 10^{-1}	(2.76±0.28) x 10^{-1}	1.03±0.16
11.00	[0.40-1.00] x 10^{-1}	(1.70±0.20) x 10^{-1}	1.19±0.11
11.50	[0.95-2.00] x 10^{-1}	(1.08±0.08) x 10^{-1}	1.20±0.12
12.00	[0.95-2.00] x 10^{-1}	(9.00±0.70) x 10^{-2}	0.93±0.10
12.40	[1.00-2.00] x 10^{-1}	(8.60±0.80) x 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] k, 10^2 $M^{-1}s^{-1}$	pH=7.1[1] k, 10^1 $M^{-1}s^{-1}$	pH=9.2[1] k, 10^0 $M^{-1}s^{-1}$
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