CONCEPT: EDTA

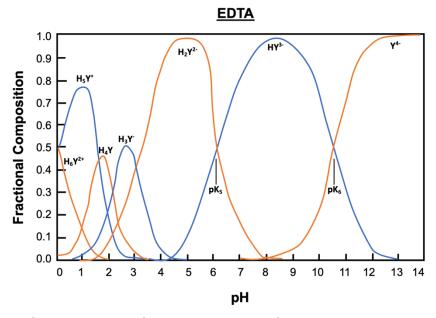
In its fully protonated form EDTA exists as a hexaprotic acid: _____

$$\begin{array}{c} :O: \\ :O: \\ :O: \\ :O: \\ :O: \\ :O: \\ \\$$

In order to form metal-complexes these acidic hydrogens must first be lost.

EDTA can exist in up to 7 different forms depending on the pH of the solution.

$$H_{6}Y^{2+} \xrightarrow{-H^{+}} H_{5}Y^{+} \xrightarrow{-H^{+}} H_{4}Y \xrightarrow{-H^{+}} H_{3}Y^{-} \xrightarrow{-H^{+}} H_{2}Y^{2-} \xrightarrow{-H^{+}} HY^{3-} \xrightarrow{-H^{+}} Y^{4-}$$



To calculate the fraction of EDTA in its basic form we can utilize the following equation:

$$\alpha_{Y^{4-}} = \frac{[Y^{4-}]}{[EDTA]} = \frac{[Y^{4-}]}{[H_6Y^{2+}] + [H_5Y^+] + [H_4Y] + [H_3Y^-] + [H_2Y^{2-}] + [HY^{3-}] + [HY^{4-}]}$$

$$\alpha_{Y^{+-}} = \frac{K_{a1}K_{a2}K_{a3}K_{a4}K_{a5}K_{a6}}{[H^{+}]^{6} + [H^{+}]^{5}K_{a1} + [H^{+}]^{4}K_{a1}K_{a2} + [H^{+}]^{3}K_{a1}K_{a2}K_{a3} + [H^{+}]^{2}K_{a1}K_{a2}K_{a3}K_{a4} + [H^{+}]K_{a1}K_{a2}K_{a3}K_{a4}K_{a5} + K_{a1}K_{a2}K_{a3}K_{a4}K_{a5} + K_{a2}K_{a3}K_{a4}K_{a5} + K_{a3}K_{a4}K_{a5} + K_{a3}K_{a5}K_{a5} + K_{a3}$$

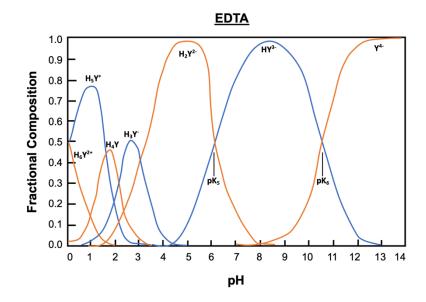
PRACTICE: EDTA CALCULATIONS 1

EXAMPLE 1: The formal concentration of EDTA is 1.50 mM. What is the concentration of the Y^{4} – form at a pH of 5.0?

pН	$\alpha_{\mathrm{Y}^{4-}}$
0	1.3×10^{-23}
1	1.4×10^{-18}
2	2.6×10^{-14}
3	2.1×10^{-11}
4	3.0×10^{-9}
5	2.9×10^{-7}
6	1.8×10^{-5}
7	3.8×10^{-4}
8	4.2×10^{-3}
9	0.041
10	0.30
11	0.81
12	0.98
13	1.00
14	1.00
* 25 °C and μ = 0	0.10 M

EXAMPLE 2: Determine the $\alpha_{Y^{4-}}$ for EDTA when the pH = 8.50.

PRACTICE: Determine the pH where $\,^{\,\Omega}_{Y^{4-}}$ equals 0.20.



CONCEPT: EDTA COMPLEXES

The _____ represents the equilibrium constant for the reaction between a ligand and a metal.

$$M^{n+} + Y^{4-} \longrightarrow MY^{n-4}$$
 $K_f = \frac{[MY^{n-4}]}{[M^{n+}][Y^{4-}]}$

The formation constants for metal-EDTA complexes are given below:

lon	logK _f	lon	logK _f	lon	logK _f
Li ⁺ Na ⁺ K ⁺ Be ²⁺ Mg ²⁺ Ca ²⁺ Sr ²⁺ Ba ²⁺ Ra ²⁺ Sc ³⁺ Y ³⁺ La ³⁺ V ²⁺ Cr ²⁺ Mn ²⁺ Fe ²⁺	2.95 1.86 0.8 9.7 8.79 10.65 8.72 7.88 7.4 23.1 ^a 18.08 15.36 12.7 ^a 13.6 ^a 13.89 14.30	V ³⁺ Cr ³⁺ Mn ³⁺ Fe ³⁺ Co ³⁺ Zr ⁴⁺ Hf ⁴⁺ VO ²⁺ VO ₂ ⁺ Ag ⁺ Tl ⁺ Pd ²⁺ Zn ²⁺ Cd ²⁺ Hg ²⁺ Sn ²⁺	25.9 ^a 23.4 ^a 25.2 25.1 41.4 29.3 29.5 18.7 15.5 7.20 6.41 25.6 ^a 16.5 16.5 21.5 18.3 ^b	Tl ³⁺ Bi ³⁺ Ce ³⁺ Pr ³⁺ Nd ³⁺ Pm ³⁺ Sm ³⁺ Eu ³⁺ Gd ³⁺ Tb ³⁺ Dy ³⁺ Ho ³⁺ Er ³⁺ Tm ³⁺ Yb ³⁺	35.3 27.8 ^a 15.93 16.30 16.51 16.9 17.06 17.25 17.35 17.87 18.30 18.56 18.89 19.32 19.49
Co ²⁺ Ni ²⁺ Cu ²⁺ Ti ³⁺	16.45 18.4 18.78 21.3	Pb ²⁺ Al ³⁺ Ga ³⁺ In ³⁺	18.0 16.4 21.7 24.9	Lu ³⁺ Th ⁴⁺ U ⁴⁺	19.74 23.2 25.7

a: 20 °C and μ = 0.1 M b: 20 °C and μ = 1.0 M

Only a portion of EDTA exists in its basic form and the lower the pH the more the other forms predominate.

$$[Y^{4-}] = \alpha_{Y^{4-}}[EDTA]$$

Under a fixed pH, $\alpha_{Y^{4-}}$ becomes a constant and can be used in determining the conditional formation constant because it represents the formation of MY^{n-4} at any pH value.

$$M^{n+} + EDTA \longrightarrow MY^{n-4}$$
 $K_f = \frac{[MY^{n-4}]}{[M^{n+}][EDTA]}$

EXAMPLE: Find $[Ba^{2+}]$ in 0.10 M BaY^{2-} at pH = 10.00.

PRACTICE: EDTA COMPLEXES CALCULATIONS 1
EXAMPLE 1: Determine the conditional formation constant for Co(EDTA) ⁻ at pH = 8.00.
EXAMPLE 2: Find the concentration of free Sn^{2+} in 0.20 M K ₂ [$Sn(EDTA)$] at pH = 9.00.
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EXAMPLE 2: Find the concentration of free Sn ²⁺ in 0.20 M K ₂ [Sn(EDTA)] at pH = 9.00.
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PRACTICE: Find the concentration of free Na⁺ in 0.15 M Li₃[Na(EDTA)] at pH = 10.00.