

- A. Calculate the fraction of each Cd^{+2} containing species and the average number of ligands gained for an uncomplexed iodide concentration of 0.0550 M.
- B. If the total cadmium concentration in A is 0.100 M, find the total iodide concentration.
- C. Prepare a distribution diagram for I^- with Cd^{+2} . Label each curve with the chemical formula of the species it represents.
- D. Calculate the molarity of each silver containing species for a total Ag^+ concentration of 1.00×10^{-4} M in a pH 8.00 solution that contains 0.10 M total NH_3 .
- E. What is the value of $[\text{Zn}^{+2}]$ in a solution containing 1.4×10^{-6} M total zinc and 1.0×10^{-5} M total ethanediamine at pH 8.50?
- F. What is the molarity of each species present in a solution containing 0.020 M Hg^{+2} and 0.30 M ammonia at pH 8.70?
- G. What is the molarity of each species present in a solution containing 0.0132 M Pb^{+2} and 0.50 M acetic acid at pH 3.50?
- H. Plot the $-\log$ of the free metal concentration as a function of the fraction titrated for the titration of 0.0010 M Co^{+2} with 0.0020 M EDTA^{-4} in the presence of 0.30 M NH_3 and 0.10 M NH_4Cl .

A. We are given $\frac{[L]}{\alpha_n} = 0.0550$. Since HI is a

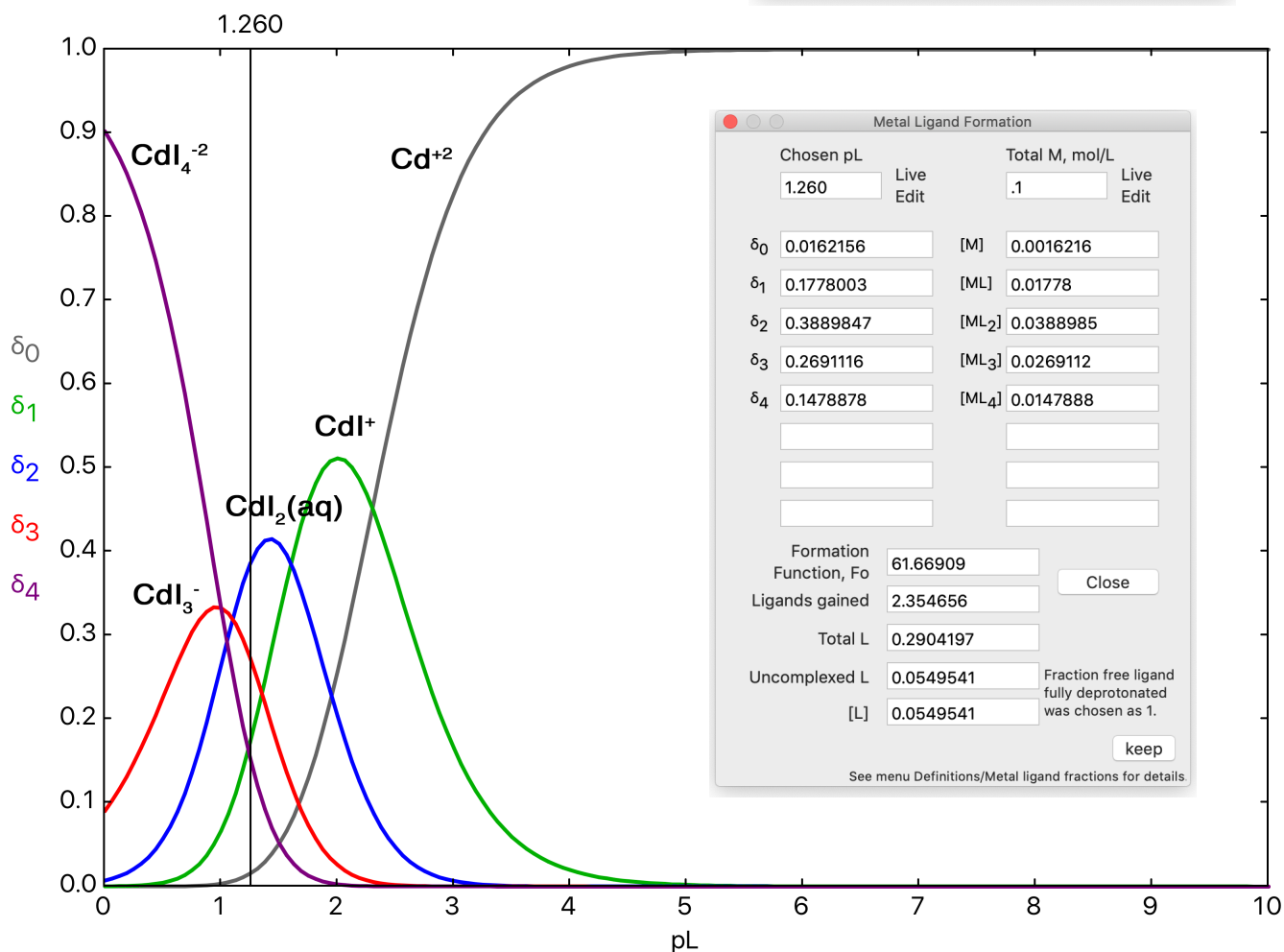
strong monoprotic acid, $\alpha_1 = 1$ (otherwise use the pH to solve for α_n) so $[I^-] = 0.0550$ and $pL = 1.260$. For Cd^{+2} and I^- , $K_{f1} = 10^{2.3}$, $K_{f2} = 10^{1.6}$, $K_{f3} = 10^{1.1}$, $K_{f4} = 10^{1.0}$.

Solve/delta fractions (distribution plot style) and click on **Show Table** for results.

$$\delta_0 = \frac{[Cd^{+2}]}{C_M} = 0.0162, \delta_1 = \frac{[CdI^+]}{C_M} = 0.178,$$

$$\delta_2 = \frac{[CdI_2(aq)]}{C_M} = 0.389, \delta_3 = \frac{[CdI_3^-]}{C_M} = 0.269,$$

$$\delta_4 = \frac{[CdI_4^{-2}]}{C_M} = 0.148, \text{ and } \bar{n} = 2.355$$



B. If $C_M = 0.100$ M (add to upper right in window above) then the total iodide molarity is

$$C_L = \bar{n} C_M + [L]/\alpha_1 = 2.355(0.100) + 0.0550 = 0.290$$

C. *Plot/Distribution vs pL for metal Kf and label as shown above.*

D. Solve for ligand concentration.

For Ag^+ and NH_3 ,

$$K_{f1} = 10^{3.31},$$

$$K_{f2} = 10^{3.92}.$$

We are given

$$C_M = 1.00 \times 10^{-4} \text{ M},$$

$$\text{and } C_L = 0.10 \text{ M}.$$

Since NH_3 is a weak monobase,

α_n depends on

$$K_a = 10^{-9.244} \text{ and}$$

pH 8.00. Click the

first **Calc** button to find $\alpha_1 = .05394$

$$\text{so } [L] = \alpha_1(0.10)$$

$$= 0.005394 \text{ and}$$

$$pL = 2.269 \text{ as}$$

displayed on the plot.

Metal Ligand Formation Constants

Log K values (leave blank if no value)

Log K_{f1} 3.31 Total metal, mol/L 1.00e-4

Log K_{f2} 3.92 Total ligand, mol/L 0.10

Log K_{f3}

Log K_{f4}

Log K_{f5}

Log K_{f6}

Log K f

Close

Apply (keyboard = enter)

Type values or open calculate window to update

Fraction of free ligand fully deprotonated at pH 8 0.0539409 Calc Set

Buffer formation function 1 Calc pH

Plot style 1 = no effect

distribution log conc

example 1 example 2 example 3 clear help keep

Ligand Acid Dissociation Constants

Log K values (leave blank if no value)

Log K_{a1} -9.244

Log K_{a2}

Log K_{a3}

Log K_{a4}

Log K_{a5}

Log K_{a6}

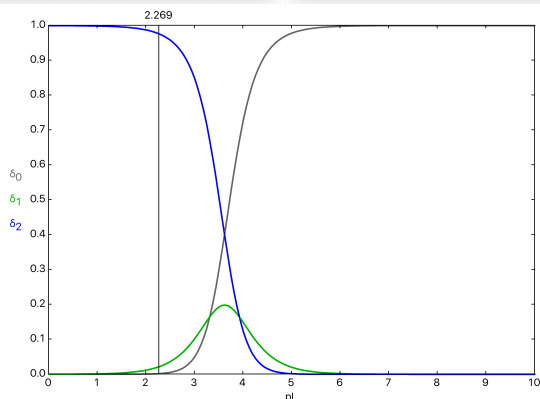
Fixed pH 8

Log K_w -14 Close

Log K f Apply (keyboard = enter)

Fraction fully deprotonated = 0.0539409

example 1 example 2 example 3 clear keep



Solve for delta

fractions with

pL = 2.269 and

click **Show Table**

$$\text{to find } [\text{Ag}^+] = \delta_0 C_M = 1.98 \times 10^{-7},$$

$$[\text{Ag}(\text{NH}_3)^+] = \delta_1 C_M = 2.18 \times 10^{-6},$$

$$[\text{Ag}(\text{NH}_3)_2^+] = \delta_2 C_M = 9.76 \times 10^{-5}.$$

Metal Ligand Formation Constants

Log K values (leave blank if no value)

Log K_{f1} 3.31

Log K_{f2} 3.92

Log K_{f3}

Log K_{f4}

Log K_{f5}

Log K_{f6}

Log K f

Close

Apply (keyboard = enter)

Type values or open calculate window to update

Fraction of free ligand fully deprotonated at pH 8.000 0.0539409 Calc Set

Buffer formation function 1 Calc pH

Plot style 1 = no effect

distribution log conc

Chosen pL 2.269 pL

Show Table

example 1 example 2 example 3 clear help keep

Metal Ligand Formation

Chosen pL 2.269 Live Edit Total M, mol/L 0.0001 Live Edit

δ_0 0.001984 [M] 1.984010e-7

δ_1 0.0218044 [ML] 2.180439e-6

δ_2 0.9762116 [ML₂] 0.0000976

Formation Function, Fo 504.0296 Close

Ligands gained 1.974228

Total L 0.0999862

Uncomplexed L 0.0997888

[L] 0.0053827

keep

See menu Definitions/Metal ligand fractions for details

E. Solve for ligand concentration.

For Zn^{+2} and en,

$$K_{f1} = 10^{5.77},$$

$$K_{f2} = 10^{5.06},$$

$$K_{f3} = 10^{3.28}.$$

We are given

$$C_M = 1.4 \times 10^{-6} \text{ M},$$

$$C_L = 1.0 \times 10^{-5} \text{ M}.$$

Since en is a weak dibase, α_n depends on $K_{a1} = 10^{-6.848}$,

$$K_{a2} = 10^{-9.928}$$

and pH 8.50. Click the first **Calc** button

to find $\alpha_2 = .03523$

and $pL = 6.464$ at the top of the graph.

Metal Ligand Formation Constants

Log K values (leave blank if no value)

Log K_{f1} 5.77 Total metal, mol/L

Log K_{f2} 5.06 1.4e-6

Log K_{f3} 3.28 Total ligand, mol/L

Log K_{f4} 1.0e-5

Log K_{f5}

Log K_{f6}

Log K f

Close

Apply (keyboard = enter)

Type values or open calculate window to update

Fraction of free ligand fully deprotonated at pH 8.5 0.0352253 Calc Set pH

Buffer formation function 1 Calc

Plot style 1 = no effect

distribution log conc

example 1 example 2 example 3 clear help keep

Ligand Acid Dissociation Constants

Log K values (leave blank if no value)

Log K_{a1} -6.848

Log K_{a2} -9.928

Log K_{a3}

Log K_{a4}

Log K_{a5} Fixed pH

Log K_{a6} 8.5

Log K_w -14

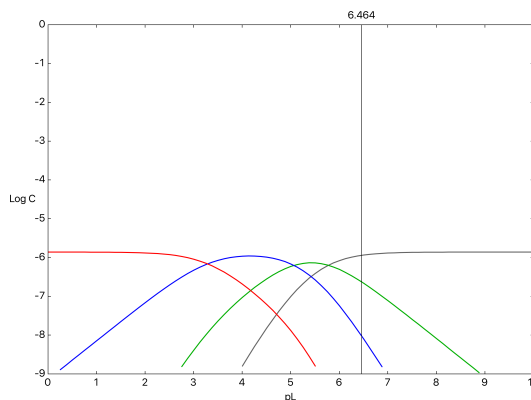
Log K f

Close

Apply (keyboard = enter)

Fraction fully deprotonated = 0.0352253

example 1 example 2 example 3 clear keep



Solve for delta

fractions and then

Show Table to find

$$[Zn^{+2}] = \delta_0 C_M =$$

$$1.16 \times 10^{-6}.$$

Metal Ligand Formation Constants

Log K values (leave blank if no value)

Log K_{f1} 5.77 Total metal, mol/L

Log K_{f2} 5.06 1.4e-6

Log K_{f3} 3.28

Log K_{f4}

Log K_{f5} Chosen pL

Log K_{f6} 6.464 pL

Log K f

Close

Apply (keyboard = enter)

Type values or open calculate window to update

Fraction of free ligand fully deprotonated at pH 8.500 0.0352253 Calc Set pH

Buffer formation function 1 Calc

Plot style 1 = no effect

distribution log conc **Show Table**

example 1 example 2 example 3 clear help keep

Metal Ligand Formation

Chosen pL 6.464 Live Edit Total M, mol/L 1.400000e-6 Live Edit

δ_0 0.8262502 [M] 1.156750e-6

δ_1 0.167152 [ML] 2.340128e-7

δ_2 0.0065934 [ML₂] 9.230807e-9

δ_3 4.316300e-6 [ML₃] 6.042820e-12

Formation Function, F_0 1.210287

Ligands gained 0.1803518

Total L 0.00001

Uncomplexed L 9.753160e-6

[L] 3.435580e-7

Close

keep

See menu Definitions/Metal ligand fractions for details.

F. *Solve for ligand concentration.*

For Hg^{+2} and NH_3 ,

$$K_{f1} = 10^{8.8},$$

$$K_{f2} = 10^{8.7},$$

$$K_{f3} = 10^{1.00},$$

$$K_{f4} = 10^{0.78}.$$

We are given

$$C_M = 0.020 \text{ M},$$

$$C_L = 0.30 \text{ M}.$$

Since NH_3 is a weak monobase, α_n depends on $K_a = 10^{-9.244}$ and pH 8.70. Click the first **Calc** button to find $\alpha_1 = .2222$ and pL = 1.256 at the top of the graph.

Solve for delta

fractions and find

$$[\text{Hg}^{+2}] = \delta_0 C_M =$$

$$1.19 \times 10^{-17},$$

$$[\text{Hg}(\text{NH}_3)^{+2}] =$$

$$\delta_1 C_M = 4.14 \times 10^{-10},$$

$$[\text{Hg}(\text{NH}_3)_2^{+2}] =$$

$$\delta_2 C_M = 0.0115,$$

$$[\text{Hg}(\text{NH}_3)_3^{+2}] =$$

$$\delta_3 C_M = 0.00638,$$

$$[\text{Hg}(\text{NH}_3)_4^{+2}] =$$

$$\delta_4 C_M = 0.00213$$

and uncomplexed ligand = 0.2496

Solve for alpha

fractions and **Show Table**

$$\text{to find } \alpha_0 \frac{[\text{L}]}{\alpha_1} =$$

$$[\text{NH}_4^+] = 0.194.$$

G. Solve for ligand concentration.

For Pb^{+2} and

CH_3COO^- ,

$K_{f1} = 10^{2.7}$,

$K_{f2} = 10^{1.4}$.

We are given

$C_M = 0.0132 \text{ M}$,

$C_L = 0.50 \text{ M}$.

Since CH_3COO^- is

a weak monobase,

α_n depends on

$K_a = 10^{-4.756}$ and

pH 3.50. Click the

first **Calc** button

to find $\alpha_1 =$

0.05255 and pL =

1.596 at the top of the graph.

Solve for delta

fractions and find

$[\text{Pb}^{+2}] = \delta_0 C_M$

$= 0.000606$,

$[\text{Pb}(\text{CH}_3\text{COO})^+] =$

$\delta_1 C_M = 0.007691$,

$[\text{Pb}(\text{CH}_3\text{COO})_2(\text{aq})] =$

$\delta_2 C_M = 0.00490$

and uncomplexed

ligand = 0.4824

Solve for alpha

fractions and find

$\alpha_0 \frac{[\text{L}]}{\alpha_1}$
 $= [\text{CH}_3\text{COOH}]$
 $= 0.457$.

Metal Ligand Formation Constants

Log K values (leave blank if no value)

Log K_{f1} 2.7 Total metal, mol/L

Log K_{f2} 1.4 0.0132

Log K_{f3} Total ligand, mol/L

Log K_{f4} 0.50

Log K_{f5}

Log K_{f6}

Log K f

Close

Apply (keyboard = enter)

Type values or open calculate window to update

Fraction of free ligand fully deprotonated at pH 3.5 0.0525481 Calc Set pH

Buffer formation function 1 Calc

Plot style 1 = no effect

distribution log conc

example 1 example 2 example 3 clear help keep

Ligand Acid Dissociation Constants

Log K values (leave blank if no value)

Log K_{a1} -4.756

Log K_{a2}

Log K_{a3}

Log K_{a4}

Log K_{a5} Fixed pH 3.50

Log K_{a6}

Log K_w -14 Close

Log K f Apply (keyboard = enter)

Fraction fully deprotonated = 0.0525481

example 1 example 2 example 3 clear keep

Metal Ligand Formation Constants

Log K values (leave blank if no value)

Log K_{f1} 2.7 Total metal, mol/L

Log K_{f2} 1.4 0.0132

Log K_{f3}

Log K_{f4}

Log K_{f5} Chosen pL 1.596 pL

Log K_{f6}

Log K f

Close

Apply (keyboard = enter)

Type values or open calculate window to update

Fraction of free ligand fully deprotonated at pH 3.500 0.0525481 Calc Set pH

Buffer formation function 1 Calc

Plot style 1 = no effect

distribution log conc Show Table

example 1 example 2 example 3 clear help keep

Metal Ligand Formation

Chosen pL 1.596 Live Edit Total M, mol/L 0.0132 Live Edit

δ_0 0.0458785 [M] 0.0006056

δ_1 0.5829204 [ML] 0.0076945

δ_2 0.3712011 [ML₂] 0.0048999

Formation Function, Fo 21.7967 Close

Ligands gained 1.325323

Total L 0.4999339

Uncomplexed L 0.4824396 [L] 0.0253513

keep

See menu Definitions/Metal ligand fractions for details.

Acid Dissociation Constants

Log K values (leave blank if no value)

Log K_{a1} -4.756 Total acid, mol/L

Log K_{a2} 0.4824396

Log K_{a3}

Log K_{a4}

Log K_{a5} Chosen pH 3.500

Log K_{a6}

Log K_w -14 Close

Log K f Apply (keyboard = enter)

Plot buffer capacity Charge on the fully protonated species 0 Examples H_2PO_4^- : 0 K_2HPO_4^- : 0 NH_4Cl : 1 NH_3 : 1 $\text{H}_3\text{NCH}_2\text{COO}^-$: 1 HCl : 0 NaOH : 0

Plot style distribution log conc Show table

example 1 example 2 example 3 clear help keep

Acid Dissociation

Chosen pH 3.500 Live Edit Total A, mol/L 0.4824396 Live Edit

α_0 0.9474519 [HA] 0.4570883

α_1 0.0525481 [A⁻] 0.0253513

Dissociation Function, Do 1.055463 Close

Protons lost 0.0525481

keep

See menu Definitions/Acid alpha fractions for details.

H. *Plot pMetal titration.* The 0.30 M NH_3 and 0.10 M NH_4Cl will act as a buffer to determine the pH. Click the **second Calc button**. Based on the K_a for NH_4^+ and the buffer concentrations the pH is 9.721. The NH_3 will also act as a ligand so enter the Co^{+2} NH_3 K_f values. The buffer formation function of ammonia with Co^{+2} is 2339. Click the **first Calc button**. The fraction of EDTA fully deprotonated at pH 9.721 depends on the K_a values for $\text{H}_4\text{EDTA}^{+2}$ and is 0.183.

Metal Ligand Formation Constants

Log K values (leave blank if no value)

Log K_{f1} 16.45 Initial metal, mol/L

Log K_{f2} 0.0010

Log K_{f3} Ligand titrant, mol/L

Log K_{f4} 0.0020

Log K_{f5} ϕ is fraction titrated

Log K_{f6} Log K mL f

Close

Apply
(keyboard = enter)

Type values or open calculate window to update

Fraction of free ligand fully deprotonated at pH 9.721 0.1832272 Calc Set

Buffer formation function 2338.997 Calc pH

1 = no effect

example 1 example 2 example 3 clear help keep

Metal and Buffer Equilibria

Log K values (leave blank if no value)

Log K_a -9.244 Buffer base form, mol/L

Log K_{f1} 1.99 0.30

Log K_{f2} 1.51 Buffer acid form, mol/L

Log K_{f3} 0.93 0.10

Log K_{f4} 0.64 Buffer pH = 9.721

Log K_{f5} 0.06 This buffer controls solution pH.

Log K_{f6} -0.74 Close

Log K f Apply
(keyboard = enter)

Buffer formation function = 2338.997

example clear keep

Ligand Acid Dissociation Constants

Log K values (leave blank if no value)

Log K_{a1} 0.00

Log K_{a2} -1.5

Log K_{a3} -2.00

Log K_{a4} -2.69

Log K_{a5} -6.13 Fixed pH

Log K_{a6} -10.37 9.721

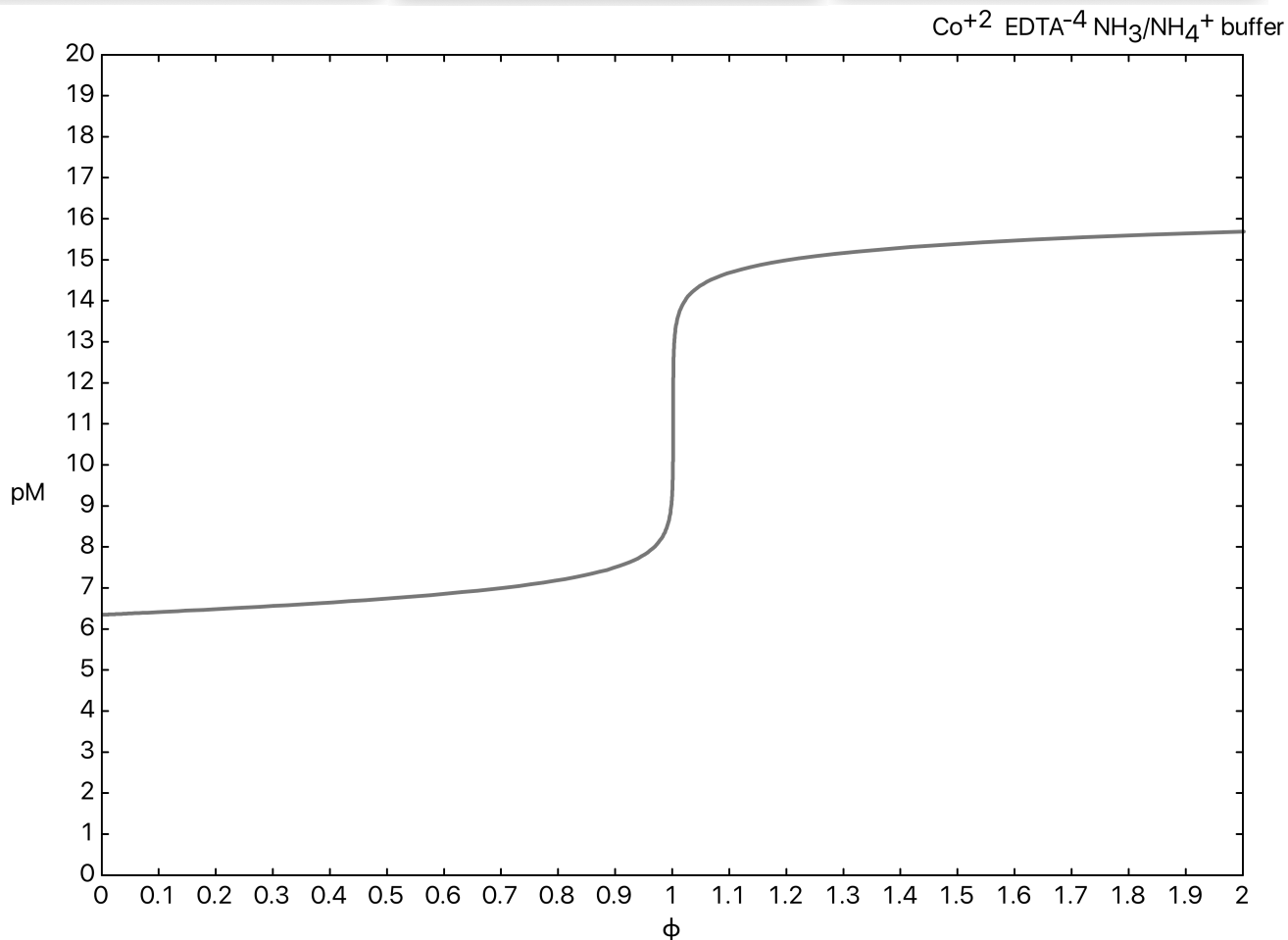
Log K_w -0.74 Solution pH controlled by buffer.

Log K f Close

Apply
(keyboard = enter)

Fraction fully deprotonated = 0.1832272

example 1 example 2 example 3 clear keep



Note: it is a helpful to use Option/Title to label your graphs.