1. Equilibrios presentes

a. Protonación del ligando

$$NH_{3(ac)} + H^+_{(ac)} \rightleftharpoons NH_4^+{}_{(ac)} \; ; \; \beta_H = 10^{9,37}$$

b. Desprotonación del quelón

$$H_4Y_{(ac)} \rightleftharpoons H_3Y^-_{(ac)} + H^+_{(ac)} \; ; \; pQa_1 = 1,99$$

$$H_3Y^-_{(ac)} \rightleftharpoons H_2Y^{2-}_{(ac)} + H^+_{(ac)} \; ; \; pQa_2 = 2,68$$

$$H_2Y^{2-}_{(ac)} \rightleftharpoons HY^{3-}_{(ac)} + H^+_{(ac)} \; ; \; pQa_3 = 6,11$$

$$HY^{3-}_{(ac)} \rightleftharpoons Y^{4-}_{(ac)} + H^+_{(ac)} \; ; \; pQa_4 = 10,17$$

c. Formación del quelato

$$Zn^{2+}_{(ac)} + Y^{4-}_{(ac)} \rightleftharpoons ZnY^{2-} \; ; \; \log Q_{ZnY} = 16,50$$

d. Formación de complejos ligando - metal

$$Zn^{2+}_{(ac)} + NH_{3(ac)} \rightleftharpoons Zn(NH_3)^{2+}_{(ac)} \; ; \; \log\beta_1 = 2,27$$

$$Zn^{2+}_{(ac)} + 2NH_{3(ac)} \rightleftharpoons Zn(NH_3)_2^{2+}{}_{(ac)} \; ; \; \log\beta_2 = 4,61$$

$$Zn^{2+}_{(ac)} + 3NH_{3(ac)} \rightleftharpoons Zn(NH_3)_3^{2+}{}_{(ac)} \; ; \; \log\beta_3 = 7,01$$

$$Zn^{2+}_{(ac)} + 4NH_{3(ac)} \rightleftharpoons Zn(NH_3)_4^{2+}{}_{(ac)} \; ; \; \log\beta_4 = 9,06$$

e. Protonación del quelato

$$ZnY^{2-}_{(ac)} + H^+_{(ac)} \rightleftharpoons ZnHY^-_{(ac)} \; ; \; \beta_{ZnHY} = 10^{3,0}$$

2. Identificación de especies

Cationes	Moléculas	Aniones
NH_4^+	NH_3	H_3Y^-
H^+	H_4Y	H_2Y^{2-}
Zn^{2+}		HY^{3-}
$Zn(NH_3)^{2+}$		Y^{4-}
$Zn(NH_3)_2^{2+}$		ZnY^{2-}
$Zn(NH_3)_3^{2+}$		$ZnHY^-$
$Zn(NH_3)_4^{2+}$		

3. Planteamiento de balances

a. Para el ligando

$$C'_L = [NH_3] + [NH_4^+] = \frac{3{,}0\,mL \cdot 3{,}20\,M}{78\,mL} = 0{,}123\,M$$

$$NH_3 + H^+ \rightleftharpoons NH_4^+ \; ; \; \beta_H = 10^{9{,}37}$$

$$\beta_H = \frac{[NH_4^+]}{[NH_3][H^+]} \therefore [NH_4^+] = \beta_H \cdot [NH_3] \cdot [H^+]$$

$$C'_L = [NH_3] + \beta_H \cdot [NH_3] \cdot [H^+]$$

$$C'_L = [NH_3](1 + \beta_H \cdot [H^+]) \therefore [NH_3] = \frac{C'_L}{(1 + \beta_H \cdot [H^+])}$$

$$[NH_3] = \frac{0{,}123\,M}{1 + 10^{9{,}37 - pH}} = 0{,}100\,M$$

4. Factores de formación

a. FHY

Reemplazando datos, se obtiene:

$$F_{HY} = 1 + 10^{pKa_4 - pH} + 10^{pKa_4 + pKa_3 - 2pH} + 10^{pKa_4 + pKa_3 + pKa_2 - 3pH} + 10^{pKa_4 + pKa_3 + pKa_2 + pKa_1 - 4pH}$$

$$F_{HY} = 2{,}48$$

b. FLM

Reemplazando datos, se obtiene:

$$F_{LM} = 1 + \beta_1 [NH_3] + \beta_2 [NH_3]^2 + \beta_3 [NH_3]^3 + \beta_4 [NH_3]^4 = 5{,}09$$

c. FMHY

Reemplazando datos, se obtiene:

$$F_{MHY} = 1 + \beta_{ZnHY} * [H^+] = 1{,}00$$

b. Para el ión metálico

$$C'_{M_L} = [Zn^{2+}] + [Zn(NH_3)^{2+}] + [Zn(NH_3)_2^{2+}] + [Zn(NH_3)_3^{2+}] + [Zn(NH_3)_4^{2+}]$$

$$\beta_1 = \frac{[Zn(NH_3)^{2+}]}{[NH_3]\cdot[Zn^{2+}]} \therefore \quad [Zn(NH_3)^{2+}] = \beta_1 \cdot [NH_3] \cdot [Zn^{2+}]$$

$$\beta_2 = \frac{[Zn(NH_3)_2^{2+}]}{[NH_3]\cdot[Zn^{2+}]} \therefore \quad [Zn(NH_3)_2^{2+}] = \beta_2 \cdot [NH_3]^2 \cdot [Zn^{2+}]$$

$$\beta_3 = \frac{[Zn(NH_3)_3^{2+}]}{[NH_3]\cdot[Zn^{2+}]} \therefore \quad [Zn(NH_3)_3^{2+}] = \beta_3 \cdot [NH_3]^3 \cdot [Zn^{2+}]$$

$$\beta_4 = \frac{[Zn(NH_3)_4^{2+}]}{[NH_3]\cdot[Zn^{2+}]} \therefore \quad [Zn(NH_3)_4^{2+}] = \beta_4 \cdot [NH_3]^4 \cdot [Zn^{2+}]$$

$$C'_{M_L} = [Zn^{2+}] + \beta_1 \cdot [NH_3][Zn^{2+}] + \beta_2 [NH_3]^2 [Zn^{2+}] + \beta_3 [NH_3]^3 [Zn^{2+}] + \beta_4 [NH_3]^4 [Zn^{2+}]$$

$$C'_{M_L} = [Zn^{2+}]\Big(\underbrace{1 + \beta_1 [NH_3] + \beta_2 [NH_3]^2 + \beta_3 [NH_3]^3 + \beta_4 [NH_3]^4}_{\text{factor ligando-metal } F_{LM}}\Big)$$

c. Para el quelón

$$C_Y = [Y^{4-}] + [HY^{3-}] + [H_2Y^{2-}] + [H_3Y^{-}] + [H_4Y]$$

$$Qa_4 = \frac{[Y^{4-}]\cdot[H^+]}{[HY^{3-}]} \therefore [HY^{3-}] = \frac{[Y^{4-}][H^+]}{Qa_4}$$

$$Qa_3 = \frac{[HY^{3-}][H^+]}{[H_2Y^{2-}]} \therefore [H_2Y^{2-}] = \frac{\frac{[Y^{4-}][H^+]}{Qa_4}\cdot[H^+]}{Qa_3} \therefore [H_2Y^{2-}] = \frac{[Y^{4-}]\cdot[H^+]^2}{Qa_4\cdot Qa_3}$$

$$Qa_2 = \frac{[H_2Y^{2-}][H^+]}{[H_3Y^-]} \therefore [H_3Y^-] = \frac{\frac{[Y^{4-}]\cdot[H^+]^2}{Qa_4\cdot Qa_3}\cdot[H^+]}{Qa_2} \therefore [H_3Y^-] = \frac{[Y^{4-}][H^+]^3}{Qa_4\cdot Qa_3\cdot Qa_2}$$

$$Qa_1 = \frac{[H_3Y^-][H^+]}{[H_4Y]} \therefore [H_4Y] = \frac{\frac{[Y^{4-}][H^+]^3}{Qa_4\cdot Qa_3\cdot Qa_2}\cdot[H^+]}{Qa_1} \therefore [H_4Y] = \frac{[Y^{4-}][H^+]^4}{Qa_4\cdot Qa_3\cdot Qa_2\cdot Qa_1}$$

$$C_Y = [Y^{4-}] + \frac{[Y^{4-}][H^+]}{Qa_4} + \frac{[Y^{4-}][H^+]^2}{Qa_4\cdot Qa_3} + \frac{[Y^{4-}][H^+]^3}{Qa_4\cdot Qa_3\cdot Qa_2} + \frac{[Y^{4-}][H^+]^4}{Qa_4\cdot Qa_3\cdot Qa_2\cdot Qa_1}$$

$$C_Y = [Y^{4-}]\left(1 + \frac{[H^+]}{Qa_4} + \frac{[H^+]^2}{Qa_4\cdot Qa_3} + \frac{[H^+]^3}{Qa_4\cdot Qa_3\cdot Qa_2} + \frac{[H^+]^4}{Qa_4\cdot Qa_3\cdot Qa_2\cdot Qa_1}\right)$$

$$C_Y = [Y^{4-}]\left(1 + \frac{10^{-pH}}{10^{-pQa_4}} + \frac{10^{-2pH}}{10^{-(pQa_4+pQa_3)}} + \frac{10^{-3pH}}{10^{-(pQa_4+pQa_3+pQa_2)}} + \frac{10^{-4pH}}{10^{-(pQa_4+pQa_3+pQa_2+pQa_1)}}\right)$$

$$C_Y = [Y^{4-}]\Big(\underbrace{1 + 10^{pQa_4-pH} + 10^{pQa_4+pQa_3-2pH} + 10^{pQa_4+pQa_3+pQa_2-3pH} + 10^{pQa_4+pQa_3+pQa_2+pQa_1-4pH}}_{\text{factor del quelón } f_{HY}}\Big)$$

d. Para los quelatos

$$C_{MYL} = [ZnY^{2-}] + [ZnHY^{-}]$$

$$\beta_{ZnHY} = \frac{[ZnHY^{-}]}{[ZnY^{2-}]\cdot[H^{+}]} \therefore [ZnHY^{-}] = \beta_{ZnHY}\cdot[ZnY^{2-}]\cdot[H^{+}]$$

$$C_{MYL} = [ZnY^{2-}] + \beta_{ZnHY}\cdot[ZnY^{2-}]\cdot[H^{+}]$$

$$C_{MYL} = [ZnY^{2-}]\left(\underbrace{1+\beta_{ZnHY}\cdot[H^{+}]}_{\substack{\text{facta de quelato} \\ f_{MYL}}}\right)$$

5. Constante condicional de establidad

$$Q'_{MY} = \frac{Q_{MY} \cdot F_{MHY}}{F_{LM} \cdot F_{HY}} \therefore Q'_{MY} = \frac{10^{16,50} \cdot 1,00}{5,09 \cdot 2,18} = 10^{9,11} > 10^{8,0}$$

6. Cálculos dependientes del punto de equivalencia

$$[\,]_{METAL} \cdot V_{METAL} = [\,]_{EDTA} \cdot V_{EDTA} \therefore V_{EDTA} = \frac{[\,]_{METAL} \cdot V_{METAL}}{[\,]_{EDTA}} = 20 mL$$

$$C_{MY} = [ZnY^{2-}] = \frac{V_{METAL} \cdot [Zn^{2+}]_i}{V_{TOTAL}} = \frac{25 mL \cdot 0{,}020 mmol}{98 mL} = 5 \times 10^{-3} M$$

$$[Zn^{2+}]_{P.E} = \sqrt{\frac{[ZnY^{2-}] \cdot f_{HY}}{Q_{ZnY} \cdot F_{LM} \cdot F_{MHY}}} \therefore [Zn^{2+}]_{P.E} = \sqrt{\frac{5 \times 10^{-3} M \cdot 2{,}48}{10^{16.5} \cdot 10^{5.09} \cdot 1{,}00}} = 1{,}78 \times 10^{-12} M$$

$$pZn_{P.E} = \log\left(\frac{1}{[Zn^{2+}]_{P.E}}\right) = 11{,}7$$

1. Equilibrios presentes

a. Protonación del ligando

$$NH_{3(ac)} + H^+_{(ac)} \rightleftharpoons NH_4^+{}_{(ac)} \; ; \; \beta_H = 10^{9,37}$$

b. Desprotonación del quelón

$$H_4Y_{(ac)} \rightleftharpoons H_3Y^-_{(ac)} + H^+_{(ac)} \; ; \; pQa_1 = 1,99$$
$$H_3Y^-_{(ac)} \rightleftharpoons H_2Y^{2-}_{(ac)} + H^+_{(ac)} \; ; \; pQa_2 = 2,68$$
$$H_2Y^{2-}_{(ac)} \rightleftharpoons HY^{3-}_{(ac)} + H^+_{(ac)} \; ; \; pQa_3 = 6,11$$
$$HY^{3-}_{(ac)} \rightleftharpoons Y^{4-}_{(ac)} + H^+_{(ac)} \; ; \; pQa_4 = 10,17$$

c. Formación del quelato

$$Zn^{2+}_{(ac)} + Y^{4-}_{(ac)} \rightleftharpoons ZnY^{4-} \; ; \; \log Q_{ZnY} = 16,50$$

d. Formación de complejos ligando - metal

$$Zn^{2+}_{(ac)} + NH_{3(ac)} \rightleftharpoons Zn(NH_3)^{2+}_{(ac)} \; ; \; \log\beta_1 = 2,27$$
$$Zn^{2+}_{(ac)} + 2NH_{3(ac)} \rightleftharpoons Zn(NH_3)^{2+}_{2\,(ac)} \; ; \; \log\beta_2 = 4,61$$
$$Zn^{2+}_{(ac)} + 3NH_{3(ac)} \rightleftharpoons Zn(NH_3)^{2+}_{3\,(ac)} \; ; \; \log\beta_3 = 7,01$$
$$Zn^{2+}_{(ac)} + 4NH_{3(ac)} \rightleftharpoons Zn(NH_3)^{2+}_{4\,(ac)} \; ; \; \log\beta_4 = 9,06$$

e. Protonación del quelato

$$ZnY^{2-}_{(ac)} + H^+_{(ac)} \rightleftharpoons ZnHY^-_{(ac)} \; ; \; \beta_{ZnHY} = 10^{3,0}$$

2. Identificación de especies

Cationes	Moléculas	Aniones
NH_4^+	NH_3	H_3Y^-
H^+	H_4Y	H_2Y^{2-}
Zn^{2+}		HY^{3-}
$Zn(NH_3)^{2+}$		Y^{4-}
$Zn(NH_3)_2^{2+}$		ZnY^{2-}
$Zn(NH_3)_3^{2+}$		$ZnHY^-$
$Zn(NH_3)_4^{2+}$		

3. Planteamiento de balances

a. Para el ligando

$$C'_L = [NH_3] + [NH_4^+] = \frac{3,0\,mL \cdot 3,20\,M}{78\,mL} = 0,123\,M$$

$$NH_3 + H^+ \rightleftharpoons NH_4^+ \; ; \; \beta_H = 10^{9,37}$$

$$\beta_H = \frac{[NH_4^+]}{[NH_3][H^+]} \therefore [NH_4^+] = \beta_H \cdot [NH_3] \cdot [H^+]$$

$$C'_L = [NH_3] + \beta_H \cdot [NH_3] \cdot [H^+]$$
$$C'_L = [NH_3](1 + \beta_H \cdot [H^+]) \therefore [NH_3] = \frac{C'_L}{(1 + \beta_H \cdot [H^+])}$$

$$[NH_3] = \frac{0,123\,M}{1 + 10^{9,37-pH}} = 0,100\,M$$

b. Para el ión metálico

$$C'_{ML} = [Zn^{2+}] + [Zn(NH_3)^{2+}] + [Zn(NH_3)_2^{2+}] + [Zn(NH_3)_3^{2+}] + [Zn(NH_3)_4^{2+}]$$

$$\beta_1 = \frac{[Zn(NH_3)^{2+}]}{[NH_3] \cdot [Zn^{2+}]} \therefore [Zn(NH_3)^{2+}] = \beta_1 \cdot [NH_3] \cdot [Zn^{2+}]$$

$$\beta_2 = \frac{[Zn(NH_3)_2^{2+}]}{[NH_3] \cdot [Zn^{2+}]} \therefore [Zn(NH_3)_2^{2+}] = \beta_2 \cdot [NH_3]^2 \cdot [Zn^{2+}]$$

$$\beta_3 = \frac{[Zn(NH_3)_3^{2+}]}{[NH_3] \cdot [Zn^{2+}]} \therefore [Zn(NH_3)_3^{2+}] = \beta_3 \cdot [NH_3]^3 \cdot [Zn^{2+}]$$

$$\beta_4 = \frac{[Zn(NH_3)_4^{2+}]}{[NH_3] \cdot [Zn^{2+}]} \therefore [Zn(NH_3)_4^{2+}] = \beta_4 \cdot [NH_3]^4 \cdot [Zn^{2+}]$$

$$C'_{ML} = [Zn^{2+}] + \beta_1 \cdot [NH_3][Zn^{2+}] + \beta_2 [NH_3]^2[Zn^{2+}] + \beta_3 [NH_3]^3[Zn^{2+}] + \beta_4 [NH_3]^4[Zn^{2+}]$$

$$C'_{ML} = [Zn^{2+}]\big(\underbrace{1 + \beta_1 [NH_3] + \beta_2 [NH_3]^2 + \beta_3 [NH_3]^3 + \beta_4 [NH_3]^4}_{\text{factor ligando - metal } F_{LM}}\big)$$

c. Para el quelón

$$C_Y = [Y^{4-}] + [HY^{3-}] + [H_2Y^{2-}] + [H_3Y^-] + [H_4Y]$$

$$Qa_4 = \frac{[Y^{4-}] \cdot [H^+]}{[HY^{3-}]} \therefore [HY^{3-}] = \frac{[Y^{4-}][H^+]}{Qa_4}$$

$$Qa_3 = \frac{[HY^{3-}][H^+]}{[H_2Y^{2-}]} \therefore [H_2Y^{2-}] = \frac{\frac{[Y^{4-}][H^+]}{Qa_4} \cdot [H^+]}{Qa_3} \therefore [H_2Y^{2-}] = \frac{[Y^{4-}] \cdot [H^+]^2}{Qa_4 \cdot Qa_3}$$

$$Qa_2 = \frac{[H_2Y^{2-}][H^+]}{[H_3Y^-]} \therefore [H_3Y^-] = \frac{\frac{[Y^{4-}] \cdot [H^+]^2}{Qa_4 \cdot Qa_3} \cdot [H^+]}{Qa_2} \therefore [H_3Y^-] = \frac{[Y^{4-}][H^+]^3}{Qa_4 \cdot Qa_3 \cdot Qa_2}$$

$$Qa_1 = \frac{[H_3Y^-][H^+]}{[H_4Y]} \therefore [H_4Y] = \frac{\frac{[Y^{4-}][H^+]^3}{Qa_4 \cdot Qa_3 \cdot Qa_2} \cdot [H^+]}{Qa_1} \therefore [H_4Y] = \frac{[Y^{4-}][H^+]^4}{Qa_4 \cdot Qa_3 \cdot Qa_2 \cdot Qa_1}$$

$$C_Y = [Y^{4-}] + \frac{[Y^{4-}][H^+]}{Qa_4} + \frac{[Y^{4-}][H^+]^2}{Qa_4 \cdot Qa_3} + \frac{[Y^{4-}][H^+]^3}{Qa_4 \cdot Qa_3 \cdot Qa_2} + \frac{[Y^{4-}][H^+]^4}{Qa_4 \cdot Qa_3 \cdot Qa_2 \cdot Qa_1}$$

$$C_Y = [Y^{4-}]\left(1 + \frac{[H^+]}{Qa_4} + \frac{[H^+]^2}{Qa_4 \cdot Qa_3} + \frac{[H^+]^3}{Qa_4 \cdot Qa_3 \cdot Qa_2} + \frac{[H^+]^4}{Qa_4 \cdot Qa_3 \cdot Qa_2 \cdot Qa_1}\right)$$

$$C_Y = [Y^{4-}]\left(1 + \frac{10^{-pH}}{10^{-pQa_4}} + \frac{10^{-2pH}}{10^{-(pQa_4 + pQa_3)}} + \frac{10^{-3pH}}{10^{-(pQa_4 + pQa_3 + pQa_2)}} + \frac{10^{-4pH}}{10^{-(pQa_4 + pQa_3 + pQa_2 + pQa_1)}}\right)$$

$$C_Y = [Y^{4-}]\big(\underbrace{1 + 10^{pQa_4 - pH} + 10^{pQa_4 + pQa_3 - 2pH} + 10^{pQa_4 + pQa_3 + pQa_2 - 3pH} + 10^{pQa_4 + pQa_3 + pQa_2 + pQa_1 - 4pH}}_{\text{factor del quelón } F_{HY}}\big)$$

d. Para los quelatos

$$C_{MYL} = [ZnY^{2-}] + [ZnHY^-]$$

$$\beta_{ZnHY} = \frac{[ZnHY^-]}{[ZnY^{2-}] \cdot [H^+]} \therefore [ZnHY^-] = \beta_{ZnHY} \cdot [ZnY^{2-}] \cdot [H^+]$$

$$C_{MYL} = [ZnY^{2-}] + \beta_{ZnHY} \cdot [ZnY^{2-}] \cdot [H^+]$$

$$C_{MYL} = [ZnY^{2-}]\big(\underbrace{1 + \beta_{ZnHY} \cdot [H^+]}_{\text{facta de quelato } F_{MYL}}\big)$$

4. Factores de formación

a. FHY

Reemplazando datos, se obtiene:

$$F_{HY} = 1 + 10^{pQa_4 - pH} + 10^{pQa_4 + pQa_3 - 2pH} + 10^{pQa_4 + pQa_3 + pQa_2 - 3pH} + 10^{pQa_4 + pQa_3 + pQa_2 + pQa_1 - 4pH}$$

$$F_{HY} = 2,48$$

b. FLM

Reemplazando datos, se obtiene:

$$F_{LM} = 1 + \beta_1 [NH_3] + \beta_2 [NH_3]^2 + \beta_3 [NH_3]^3 + \beta_4 [NH_3]^4 = 5,09$$

c. FMHY

Reemplazando datos, se obtiene:

$$F_{MHY} = 1 + \beta_{ZnHY} * [H^+] = 1,00$$

5. Constante condicional de establidad

$$Q'_{MY} = \frac{Q_{MY} \cdot F_{MHY}}{F_{LM} \cdot F_{HY}} \therefore Q'_{MY} = \frac{10^{16,50} \cdot 1,00}{5,09 \cdot 2,48} = 10^{9,11} > 10^{8,0}$$

6. Cálculos dependientes del punto de equivalencia

$$[\,]_{METAL} \cdot V_{METAL} = [\,]_{EDTA} \cdot V_{EDTA} \therefore V_{EDTA} = \frac{[\,]_{METAL} \cdot V_{METAL}}{[\,]_{EDTA}} = 20\,mL$$

$$C_{MY} = [ZnY^{2-}] = \frac{V_{METAL} \cdot [Zn^{2+}]_i}{V_{TOTAL}} = \frac{25\,mL \cdot 0,020\,mmol}{98\,mL} = 5 \times 10^{-3}\,M$$

$$[Zn^{2+}]_{P.E} = \sqrt{\frac{[ZnY^{2-}] \cdot F_{HY}}{Q_{ZnY} \cdot F_{LM} \cdot F_{MHY}}} \therefore [Zn^{2+}]_{P.E} = \sqrt{\frac{5 \times 10^{-3}\,M \cdot 2,48}{10^{16,5} \cdot 10^{5,09} \cdot 1,00}} = 1,78 \times 10^{-12}\,M$$

$$pZn_{P.E} = \log\left(\frac{1}{[Zn^{2+}]_{P.E}}\right) = 11,7$$