Tenim una dissolució en la que la concentració inicial de $[F^-]_0 = 0.5$ M i la de $[Sn^{+2}]_0 = 0.05$ M. Determineu les concentracions de F^-, Sn^{+2} i de tots els compostos de coordinació una volta assolit l' equilibri a partir de les dades seguents :
SnF^+ Log $\beta_1 = 4.1$, SnF_2 Log $\beta_2 = 6.7$, SnF_3^- Log $\beta_3 = 9.5$,

In[95]:= **ClearAll["Global`*"]**

In[96]:=
$$cm = 0.05;\ cl = 0.5;\ \beta 1 = 10^{4.1};\ \beta 2 = 10^{6.7};\ \beta 3 = 10^{9.5};$$
$$sol = Solve\left[\left\{\beta 1 == \frac{ml}{m\ l},\ \beta 2 == \frac{ml2}{m\ l^2},\ \beta 3 == \frac{ml3}{m\ l^3},\ cl == l + ml + 2\ ml2 + 3\ ml3,\ cm == m + ml + ml2 + ml3\right\},\ \{m, l, ml, ml2, ml3\}\right]$$

Out[97]=
$$\{\{ml \to -0.180796 - 0.0817063\,i,\ ml2 \to -0.00481544 + 0.17582\,i,\ ml3 \to 0.230429 - 0.0892932\,i,\ m \to 0.00518178 - 0.00482026\,i,\ l \to -0.000861161 - 0.00205357\,i\},$$
$$\{ml \to -0.180796 + 0.0817063\,i,\ ml2 \to -0.00481544 - 0.17582\,i,\ ml3 \to 0.230429 + 0.0892932\,i,\ m \to 0.00518178 + 0.00482026\,i,\ l \to -0.000861161 + 0.00205357\,i\},$$
$$\{ml \to 1.61544 \times 10^{-6},\ ml2 \to 0.000225239,\ ml3 \to 0.0497731,\ m \to 3.66648 \times 10^{-10},\ l \to 0.350228\},$$
$$\{ml \to 0.535569,\ ml2 \to -0.0194116,\ ml3 \to 0.00111508,\ m \to -0.467272,\ l \to -0.0000910427\}\}$$

In[98]:= **sol[[3]]**

Out[98]=
$$\{ml \to 1.61544 \times 10^{-6},\ ml2 \to 0.000225239,\ ml3 \to 0.0497731,\ m \to 3.66648 \times 10^{-10},\ l \to 0.350228\}$$

In[100]:=
$$L = cl - 3\ cm;\ Print["L = ", L];\ M = \frac{cm}{1 + \beta 1\ L + \beta 2\ L\hat{}2 + \beta 3\ L\hat{}3};\ Print["M = ", M]$$

L = 0.35

M = 3.67104×10^{-10}

In[101]:= $k1 = \beta 1;\ k2 = \beta 2 / \beta 1;\ k3 = \beta 3 / \beta 2;$

In[102]:=
$$sol1 = Solve\left[k1 == \frac{ML}{M\ L},\ ML\right]$$

Out[102]= $\{\{ML \to 1.61755 \times 10^{-6}\}\}$

In[103]:=
$$ML = sol1[[1, 1, 2]];\ sol2 = Solve\left[k2 == \frac{ML2}{ML\ L},\ ML2\right]$$

Out[103]= $\{\{ML2 \to 0.000225385\}\}$

In[104]:=
$$ML2 = sol2[[1, 1, 2]];\ sol3 = Solve\left[k3 == \frac{ML3}{ML2\ L},\ ML3\right]$$

Out[104]= $\{\{ML3 \to 0.049773\}\}$

$[L]_0 = C_L = 0.5$ $\quad$ $\beta_1 = 10^{4.1} = \frac{[ML]}{[M][L]}$ $\quad$ $\beta_2 = 10^{6.7} = \frac{[ML_2]}{[M][L]^2}$ $\quad$ $\beta_3 = \frac{[ML_3]}{[M][L]^3} = 10^{9.5}$

$[M]_0 = C_M = 0.05$

BALANÇOS $\begin{cases} C_M = M + ML + ML_2 + ML_3 & [1] \\ C_L = L + ML + 2ML_2 + 3ML_3 & [2] \end{cases}$

Com $3C_L < C_M$ si la formació de ML_3 se completa $M \to 0$ i "sobra" L

$\begin{cases} \text{La mínima quantitat possible de } [L] = C_L - 3C_M = 0.35M \text{ (reacció completa)} \\ \text{La màxima quantitat possible de } [L] = C_L = 0.5M \text{ (no hi ha reacció)} \end{cases}$

En qualsevol dels casos límits (i el cas real és $0.5 < [L] < 0.35$) tenim que:

β_1 ens diu que $[ML] \sim 4 \cdot 10^4 [M]$ i.e $[ML] \gg [M]$

$$k_2 = \frac{\beta_2}{\beta_1} = \frac{[ML_2]}{[L][ML]} = 10^{2.6} \rightarrow [ML_2] \sim 4 \cdot 10^{1.6} [ML] \Rightarrow [ML_2] \gg [ML]$$

$$k_3 = \frac{\beta_3}{\beta_2} = \frac{[ML_3]}{[L][ML_2]} = 10^{2.8} \rightarrow [ML_3] \sim 4 \cdot 10^{1.8} [ML_2] \Rightarrow [ML_3] \gg [ML_2]$$

(i) Aproximació més grossera: $\quad M = ML = ML_2 = 0$

$$\left.\begin{array}{l} \text{Desde } [1] \rightarrow \boxed{C_M = ML_3} \\ \text{Desde } [2] \rightarrow C_L = L + 3ML_3 \rightarrow L = C_L - 3C_M \end{array}\right\} \text{portant-ho a } \beta_3$$

$\hookrightarrow L = 0.35M$

$$\beta_3 = 10^{9.5} = \frac{C_M}{M(C_L - 3C_M)^3} = \frac{0.05}{M\, 0.35^3} \rightarrow M = 3.688 \cdot 10^{-10} M$$

$$\text{portant-ho a } \beta_1 = 10^{4.1} = \frac{ML}{ML} = \frac{ML}{3.688 10^{-10} * 0.35} \rightarrow ML = 1.625 \cdot 10^{-6} M$$

$$\text{portant ho a } \beta_2 = 10^{6.7} = \frac{ML_2}{ML^2} = \frac{ML_2}{3.688 \cdot 10^{-10}\, 0.35^2} \rightarrow ML_2 = 0.000226 \quad M$$

$$\text{portant-ho a } \beta_3 = 10^{9.5} = \frac{ML_3}{ML^3} = \frac{ML_3}{3.688 \cdot 10^{-10}\, 0.35^3} \rightarrow ML_3 = 0.05$$

(ii) Aproximació menys severa $M = ML \simeq 0 \Rightarrow$ Els balanços són ara

$$\left.\begin{array}{l} C_M = ML_2 + ML_3 \\ C_L = L + 2ML_2 + 3ML_3 \end{array}\right\} \begin{array}{ll} C_L - 2C_M = L + ML_3 \rightarrow ML_3 = C_L - 2C_M - L & [3] \\ C_L - 3C_M = L - ML_2 \rightarrow ML_2 = L - C_L + 3C_M & [4] \end{array}$$

$$\frac{\beta_2 = \dfrac{ML_2}{\cancel{M}\,\cancel{L^2}}}{\beta_3 = \dfrac{ML_3}{\cancel{M}\,\cancel{L^3}}} \qquad \frac{\beta_2}{\beta_3} = \frac{ML_2 \cdot L}{ML_3} = \frac{(L - C_L + 3C_M)L}{C_L - 2C_M - L}$$ eq. de segon grau

$\rightarrow L = 0.350225\,M$ (rebutgem $L < 0$)

Desde [3] $ML_3 = 0.049775\,M$

Desde [2] $ML_2 = 0.000225\,M$

Desde $\beta_2 \rightarrow M = 3.664 \cdot 10^{-10}\,M$

Desde $\beta_3 \rightarrow M = 3.664 \cdot 10^{-10}\,M$ ok

Desde $\beta_1 \rightarrow ML = \beta_1 M L = 1.616 \cdot 10^{-6}\,M$

(iii) Si fem aproximacions menys severes ja no trobem eqs de 2^{on} grau

La solució exacta sense rebutjar res al costat de les aproximacions

	severa	menys severa	exacte
M	$3.688 \cdot 10^{-10}$	$3.664 \cdot 10^{-10}$	$3.667 \cdot 10^{-10}$
L	0.35	0.350225	0.350228
ML	$1.625 \cdot 10^{-6}$	$1.616 \cdot 10^{-6}$	$1.615 \cdot 10^{-6}$
ML_2	0.000226	0.000225	0.000225
ML_3	0.05	0.049775	0.049773