



M = metal

S = substrate (18CG)

C = M.S (complex)

$$K_S = \frac{[C]}{[M][S]}$$

$$d_{obs} = d_F X_F + d_C X_C$$

$d_C, d_F =$ chem shifts

$$X_F = \frac{M}{M+C}$$

$$X_C = 1 - X_F$$

$X_{F,C} =$ molar fraction

Let $d_F = 0$

$$\therefore d_{obs} = d_C X_C + \cancel{d_F X_F} \rightarrow 0$$

$$= d_C [1 - X_F]$$

$$= d_C \left[1 - \frac{M}{M+C} \right]$$

$$d_{obs} = d_C - d_C \left(\frac{M}{M+C} \right)$$

$$d_C - d_{obs} = d_C \left(\frac{M}{M+C} \right)$$

$$f_C - f_{OBS} = f_C \left(\frac{M}{M+C} \right) \quad \left. \vphantom{f_C - f_{OBS}} \right\} \text{rearrange} \quad \textcircled{2}$$

$$(f_C - f_{OBS})(M+C) = f_C M$$

$$f_C M + f_C C - f_{OBS} M - f_{OBS} C = f_C M \quad \left. \vphantom{f_C M + f_C C} \right\} \neq \frac{1}{M \cdot S}$$

$$\frac{f_C M}{MS} + \frac{f_C C}{MS} - \frac{f_{OBS} M}{MS} - \frac{f_{OBS} C}{MS} = \frac{f_C M}{MS}$$

$$\cancel{\frac{f_C}{S}} + \frac{f_C C}{MS} - \frac{f_{OBS}}{S} - \frac{f_{OBS} C}{MS} = \cancel{\frac{f_C}{S}}$$

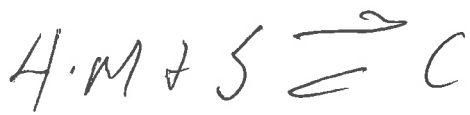
$$\frac{f_{OBS} C}{MS} \neq \frac{f_{OBS}}{S} = \frac{f_C C}{MS}$$

$$\boxed{\frac{f_{OBS}}{S} = -\frac{f_{OBS} C}{MS} + \frac{f_C C}{MS}}$$

$$K_S = \frac{C}{MS} \quad M+S \Rightarrow C$$

$$\therefore \boxed{\frac{f_{OBS}}{S} = -f_{OBS} K_S + f_C K_S}$$

$$y = mx + b$$



$M = \text{Metal}$

$S = \text{Substrate}$

$C = \text{Complex}$

①

$$K_S = \frac{[C]}{[M]^4 S}$$

$$d_{obs} = d_F X_F + d_C X_C$$

$$X_F = \frac{[M]^4}{[M]^4 + [C]}$$

$$X_C = 1 - X_F$$

Let $d_F = 0$

$$d_{obs} = \cancel{d_F X_F} + d_C X_C$$

$$d_{obs} = d_C [1 - X_F]$$

$$d_{obs} = d_C - d_C \left[\frac{M^4}{M^4 + C} \right]$$

$$d_C - d_{obs} = d_C \left[\frac{M^4}{M^4 + C} \right]$$

rearrange

$$(d_C - d_{obs})(M^4 + C) = d_C M^4$$

$$d_C M^4 + d_C C - d_{obs} M^4 - d_{obs} C = d_C M^4$$

$$f_c M^4 + f_c C - f_{obs} M^4 - f_{obs} C = f_c M^4 \quad \textcircled{2}$$

$$\frac{f_c M^4 + f_c C}{M^4 S} - \frac{f_{obs} M^4 - f_{obs} C}{M^4 S} = \frac{f_c M^4}{M^4 S}$$

$$\frac{f_c}{S} + \frac{f_c C}{M^4 S} - \frac{f_{obs}}{S} - \frac{f_{obs} C}{M^4 S} = \frac{f_c}{S}$$

$$\frac{f_{obs}}{S} = -\frac{f_{obs} C}{M^4 S} + \frac{f_c C}{M^4 S}$$

$$K_S = \frac{C}{M^4 S}$$

$$\frac{f_{obs}}{S} = -f_{obs} K_S + f_c K_S$$

$$y = mx + b$$



①

$$K_s = \frac{C}{MS^{1/4}}$$

$$d_{\text{OBS}} S = d_F X_F + d_C X_C$$

$$X_F = \frac{M}{M+C}$$

$$X_C = 1 - X_F$$

$$d_{\text{OBS}} S = d_C (1 - X_F) = d_C - \frac{d_C M}{M+C}$$

$$d_C - d_{\text{OBS}} S = \frac{d_C M}{M+C}$$

$$(d_C - d_{\text{OBS}} S)(M+C) = d_C M$$

$$d_C M + d_C C - d_{\text{OBS}} S M - d_{\text{OBS}} S C = d_C M \quad \} \times \frac{1}{MS^{1/4}}$$

$$\frac{d_C M}{MS^{1/4}} + \frac{d_C C}{MS^{1/4}} - \frac{d_{\text{OBS}} S M}{MS^{1/4}} - \frac{d_{\text{OBS}} S C}{MS^{1/4}} = \frac{d_C M}{MS^{1/4}}$$

$$\frac{d_C}{S^{1/4}} + \frac{d_C C}{MS^{1/4}} - \frac{d_{\text{OBS}} S}{S^{1/4}} - \frac{d_{\text{OBS}} S C}{MS^{1/4}} = \frac{d_C}{S^{1/4}}$$

$$\frac{f_c c}{MS^{1/4}} - \frac{\delta_{obs}}{S^{1/4}} - \frac{\delta_{obs} c}{MS^{1/4}} = 0$$

$$\frac{\delta_{obs}}{S^{1/4}} = \frac{f_c c}{MS^{1/4}} - \frac{\delta_{obs} c}{MS^{1/4}}$$

$$\frac{\delta_{obs}}{S^{1/4}} = -\frac{\delta_{obs} c}{MS^{1/4}} + \frac{f_c c}{MS^{1/4}}$$

$$K_S = \frac{c}{MS^{1/4}}$$

$$\frac{\delta_{obs}}{S^{1/4}} = -\delta_{obs} K_S + f_c K_S$$

$$y = mx + b$$