

(18.9) Calculate  $\beta_4$  and the distribution constant using (18.32) and Figure 18.9.

Use lower curve as the upper one is for very high concentration in the organic phase.

$$\text{Eqn. (18.32)} \quad D_M = K_{DC} \cdot \beta_z [A]^{z/\Sigma \beta_n [A]^n}$$

$n_{\max}$  in the sum must be 4 and  $z = 3$ .

As a first approximation assume that the denominator is dominated by the term  $\beta_3 [A]^3$  at the maximum  $D$ -value, i.e.  $\log(D_M) = 0.1$  and  $pA = 2.5$ . In this point we then have  $D_M = K_{DC}$ , i.e.  $K_{DC} = 10^{0.1}$ .

At the highest  $pA$  values the denominator is dominated by the first term in the sum, i.e.  $\beta_0 [A]^0 = 1$  per definition as  $\beta_0 = 1$ . Then we can approximate  $D_M = K_{DC} \cdot \beta_3 [A]^3$  at  $pA = 6.25$  and  $\log(D_M) = -5$ . This permits us to calculate  $\beta_3$ .

Thus the following procedure yields first approximations for  $K_{DC}$  and  $\beta_4$  that can be used as starting values for a least squares refinement.

At the maximum of the curve:

$$\log D_M := 0.1 \quad K_{DC} := 10^{\log D_M} \quad K_{DC} = 1.259$$

At  $pA = 6.25$ :

$$pA := 6.25 \quad A := 10^{-pA} \quad A = 5.623 \cdot 10^{-7}$$

$$\log D_M := -5 \quad D_M := 10^{\log D_M} \quad D_M = 1 \cdot 10^{-5}$$

$$D_M = K_{DC} \cdot \beta_3 A^3 \quad \beta_3 := \frac{D_M}{K_{DC} \cdot A^3} \quad \beta_3 = 4.467 \cdot 10^{13}$$

$$\log(\beta_3) = 13.65$$

At  $pA = 0.5$ :

$$pA := 0.5 \quad A := 10^{-pA} \quad A = 0.316$$

$$\log D_M := -1.1 \quad D_M := 10^{\log D_M} \quad D_M = 0.079$$

$$D_M = \frac{K_{DC} \cdot \beta_3 A^3}{\beta_3 A^3 + \beta_4 A^4} \quad \beta_4 := \frac{\beta_3 (K_{DC} - D_M)}{D_M A} \quad \beta_4 = 2.097 \cdot 10^{15}$$

$$\log(\beta_4) = 15.32$$