(9.9) Calculate β_4 and the distribution constant using (9.23a) and Figure 9.9.

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

Eqn. (9.23) $D_M = K_{DC}*\beta_z[A^-]^z/\Sigma\beta_n[A^-]^n$

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 β_0=1. Then we can approximate $D_M=K_{DC}*\beta_3[A-]^3$ at pA = 6.25 and log(D_M)=-5. This permits us to calculate β_3.

Thus the following procedure yields first approximations for K_{DC} and β_4 that can be used as starting values for a least squares refinement.

At the maximum of the curve:

$logD_M := 0.1$ $\qquad K_{DC} := 10^{logD_M}$ $\qquad K_{DC} = 1.259$

At pA=6.25:

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

$logD_M := -5$ $\qquad D_M := 10^{logD_M}$ $\qquad D_M = 1\cdot 10^{-5}$

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

$$log(\beta_3) = 13.65$$

At pA=0.5:

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

$logD_M := -1.1$ $\qquad D_M := 10^{logD_M}$ $\qquad D_M = 0.079$

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

$$log(\beta_4) = 15.32$$