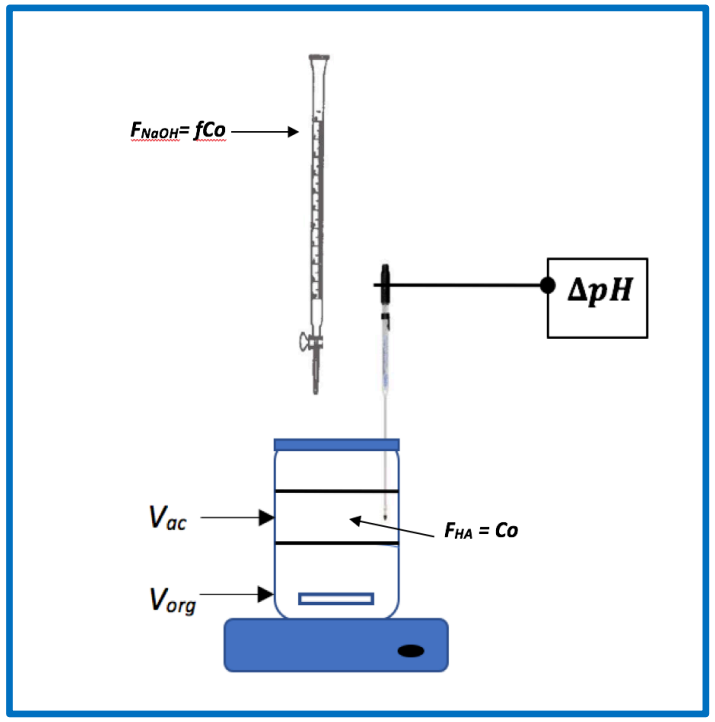
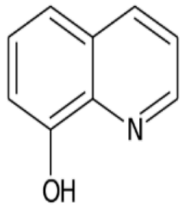


QA III
Acidez-distribución líquido-líquido
DLTED
Oxinio/oxina/oxinato
H_2O-$CHCl_3$

La oxina, *HOx*, se distribuye entre el agua y el cloroformo, $K_D = 720 \approx 10^3$, el hidrógeno fenólico es disociable, $pKa_2 = 5$ y el nitrógeno heterocíclico es protonable, $pKa_1 = 9.7 \approx 10$:



$$H_2OX^+ \rightleftharpoons \mathbf{HOX} \rightleftharpoons OX^-$$
$$\Updownarrow$$
$$\mathbf{(HOx)_{org}}$$

Diagrama pH = pKa´= f(p(Vo/Va):

$$K_D = \frac{[HOx]_{org}}{[HOX]_{ac}} = 10^3$$

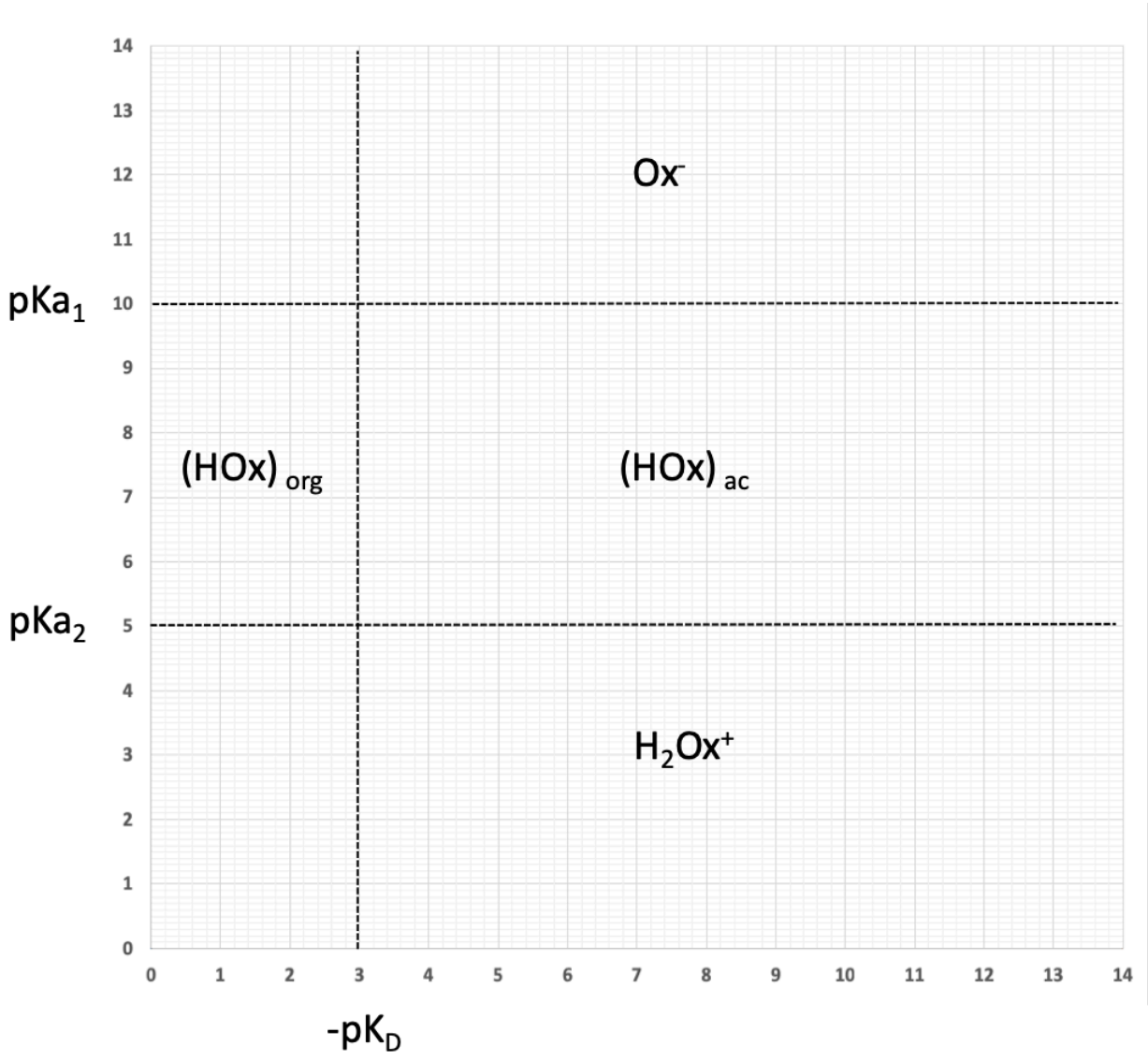
$$K_D \left(\frac{V_o}{V_a}\right) = \frac{n_{org}}{n_{ac}}$$

$$n_{org} = n_{ac}$$

$$K_D = \left(\frac{V_a}{V_o}\right) = 10^3$$

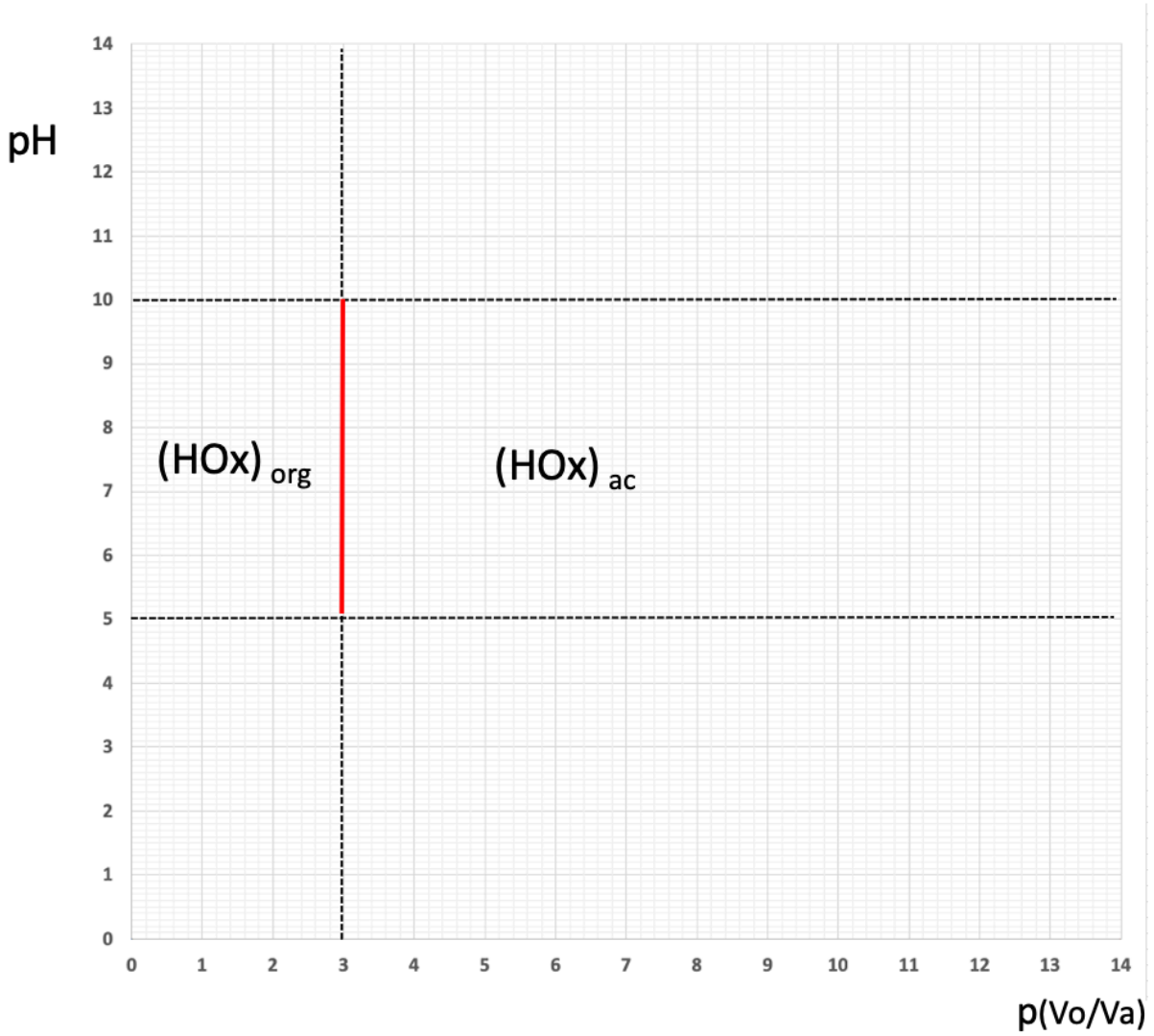
$$-\log K_D = \log \left(\frac{V_o}{V_a}\right) = -3$$

$$\log K_D = p\left(\frac{V_o}{V_a}\right) = -pK_D = 3$$



Distribución molecular:

$(HOX)_{org} \rightleftharpoons (HOX)_{ac}$



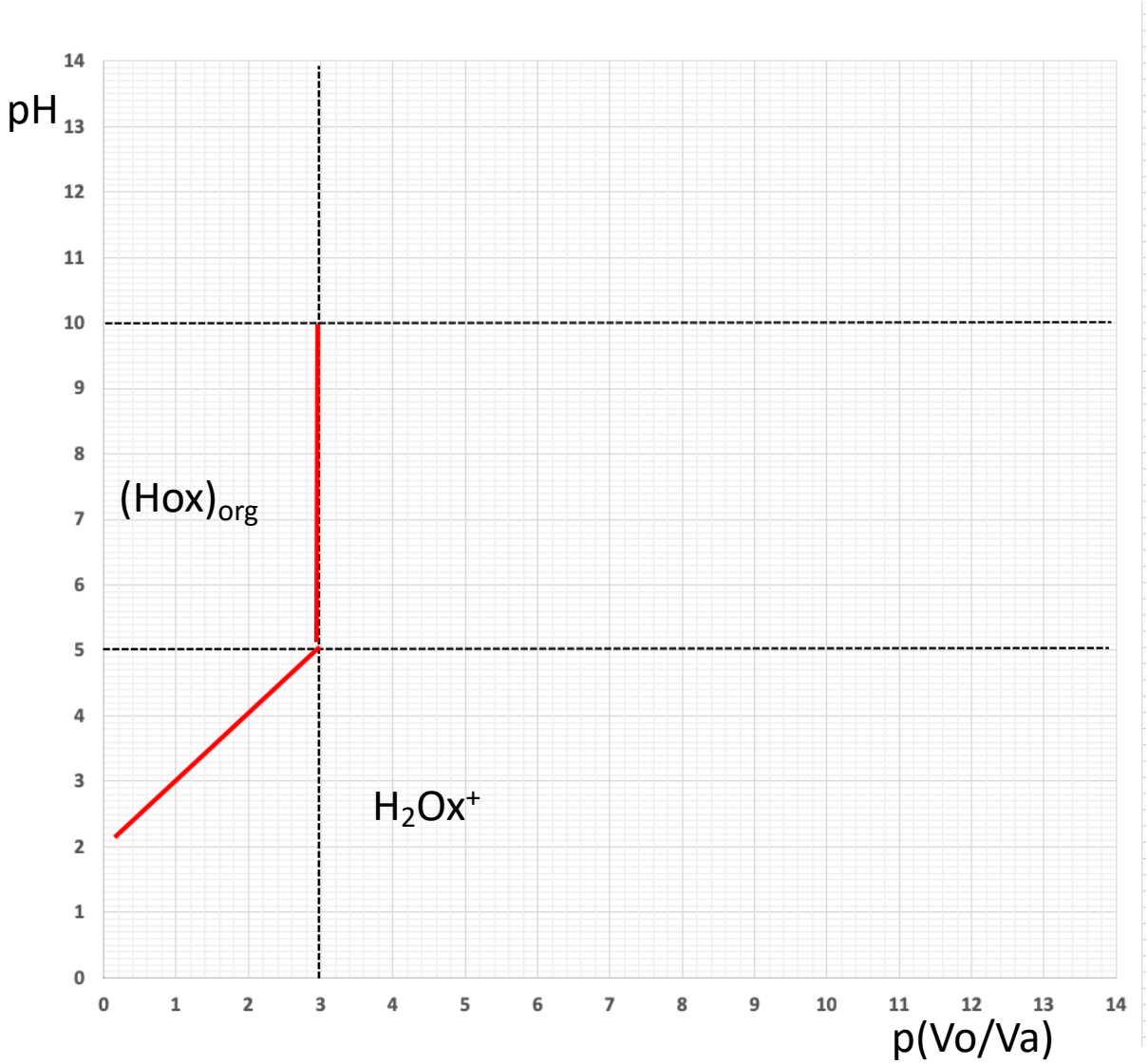
Distribución iónica ácida:

$H_2Ox^+ \rightleftharpoons (HOx)_{ac} + H^+ \quad Ka_2=10^{-5}$
$(HOx)_{ac} \rightleftharpoons (HOx)_{org} \quad K_D = 10^3$

$H_2Ox^+ \rightleftharpoons (HOx)_{org} + H^+ \quad K_{gbl} = 10^{-2}$

$$K_{gbl}\left(\frac{V_a}{V_o}\right) = \frac{n_{org}[H^+]}{n_{ac}}$$

$$pH = pKa_2' = 2 + p\left(\frac{Vo}{Va}\right)$$



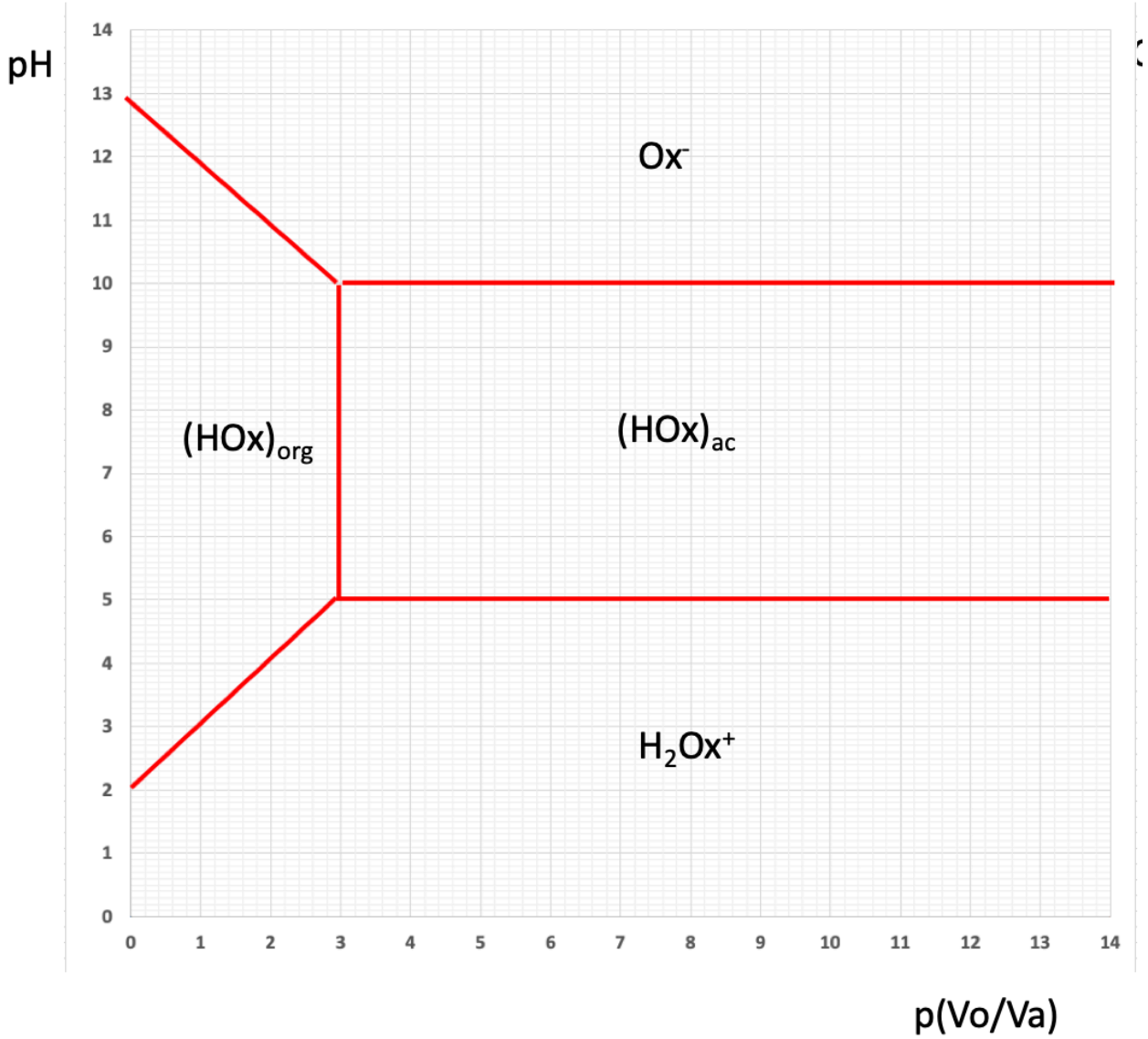
Distribución iónica alcalina:

$(HOx)_{ac} \rightleftharpoons Ox^- + H^+ \qquad Ka_2 = 10^{-10}$

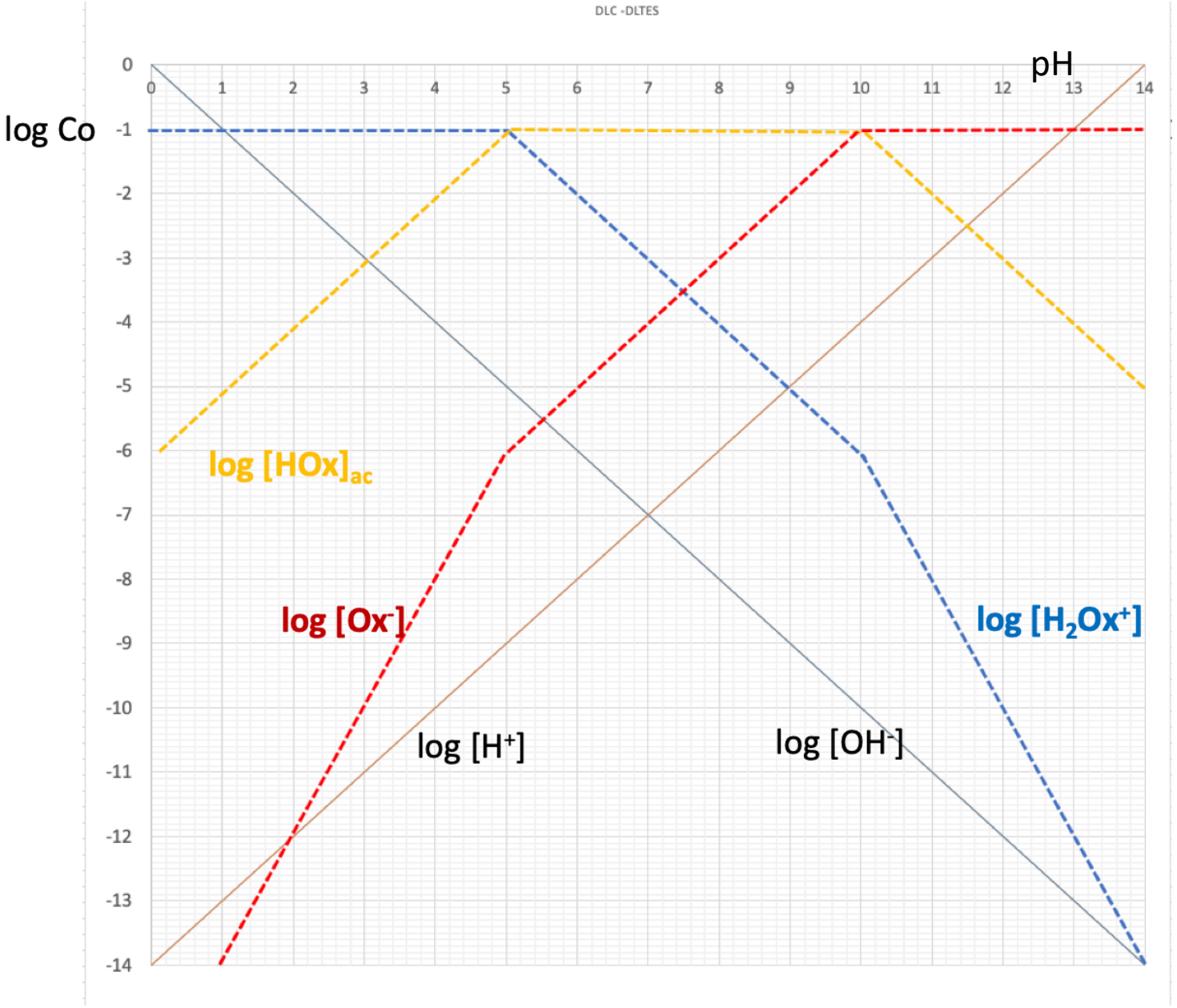
$(HOx)_{org} \rightleftharpoons (HOx)_{ac} \qquad K_D{}^{-1} = 10^{-3}$

$(HOx)_{org} \rightleftharpoons Ox^- + H^+ \qquad K_{gbl} = 10^{-13}$

$$pH = pKa_1{}' = 13 - p(\frac{Vo}{Va})$$



DLC → DLTED

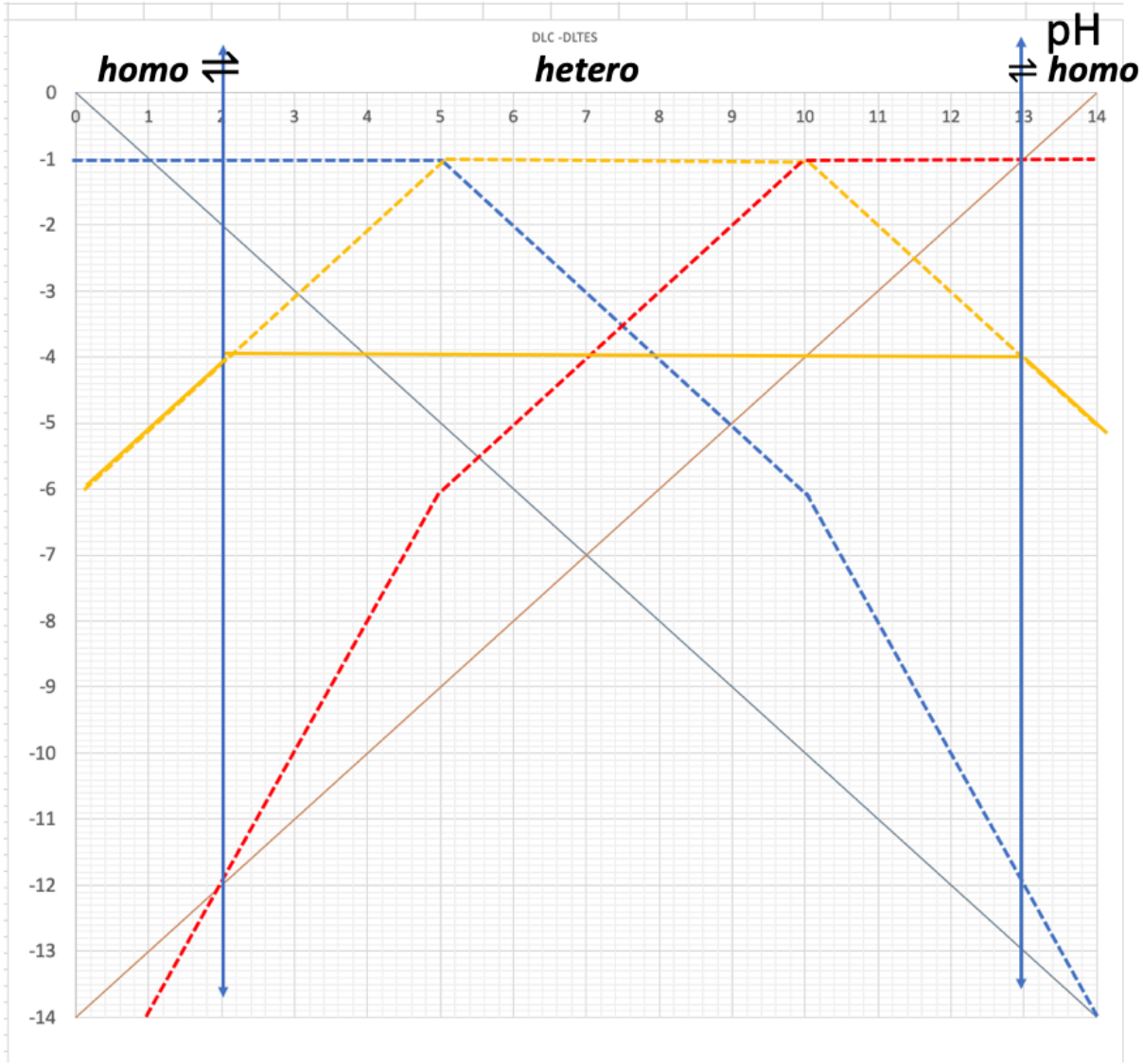

DLC -DLTES
pH
log Co
0
-1
-2
-3
-4
-5
-6
-7
-8
-9
-10
-11
-12
-13
-14
0
1
2
3
4
5
6
7
8
9
10
11
12
13
14
log [HOx]ac
log [Ox-]
log [H2Ox+]
log [H+]
log [OH-]

DLC → DLTED

Distribución molecular a p(Vo/Va) = 0

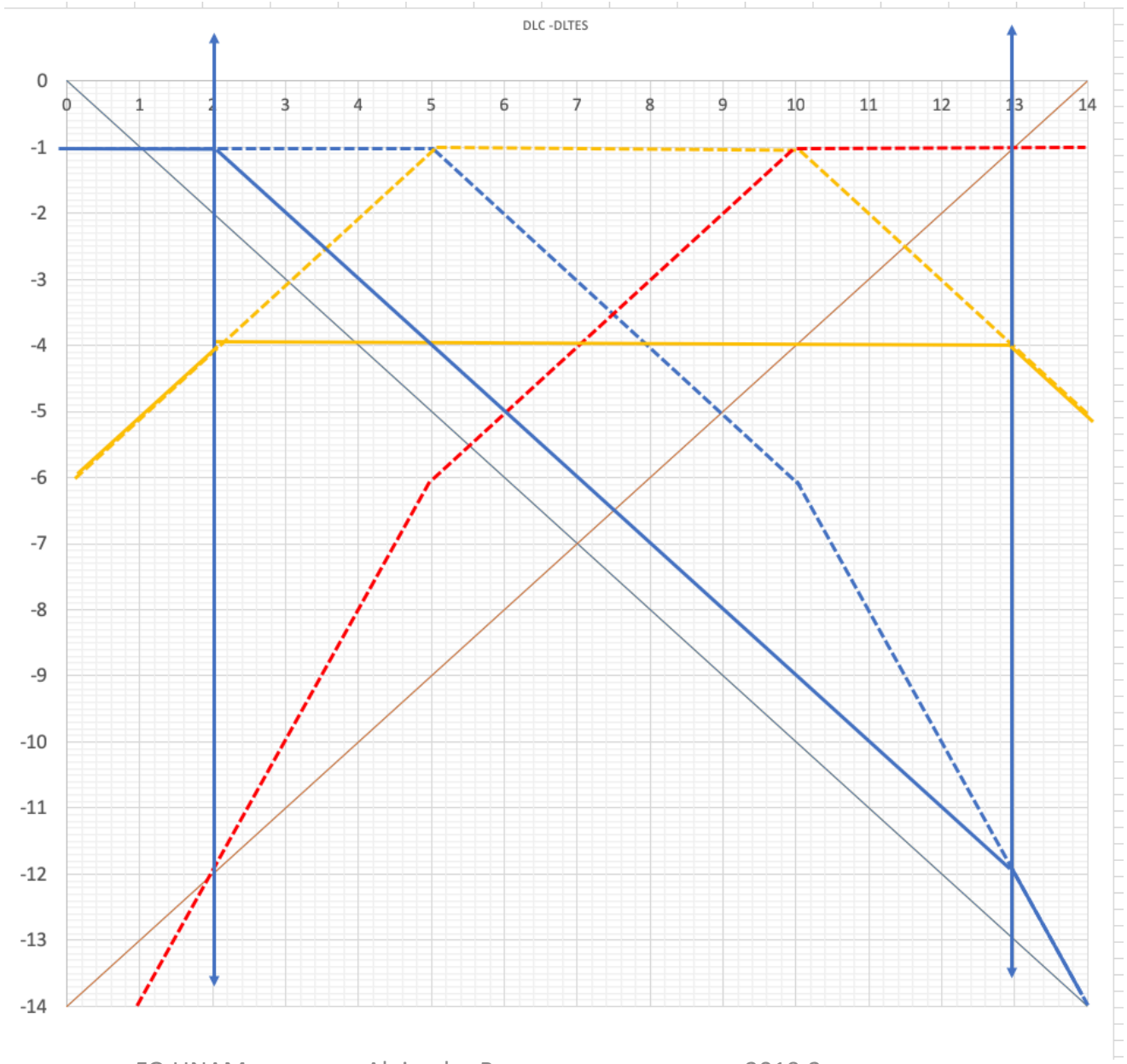
$$K_D \approx \frac{Co}{[HOx]_{ac}} = 10^3$$

$$log[HOx]_{ac} = -4$$



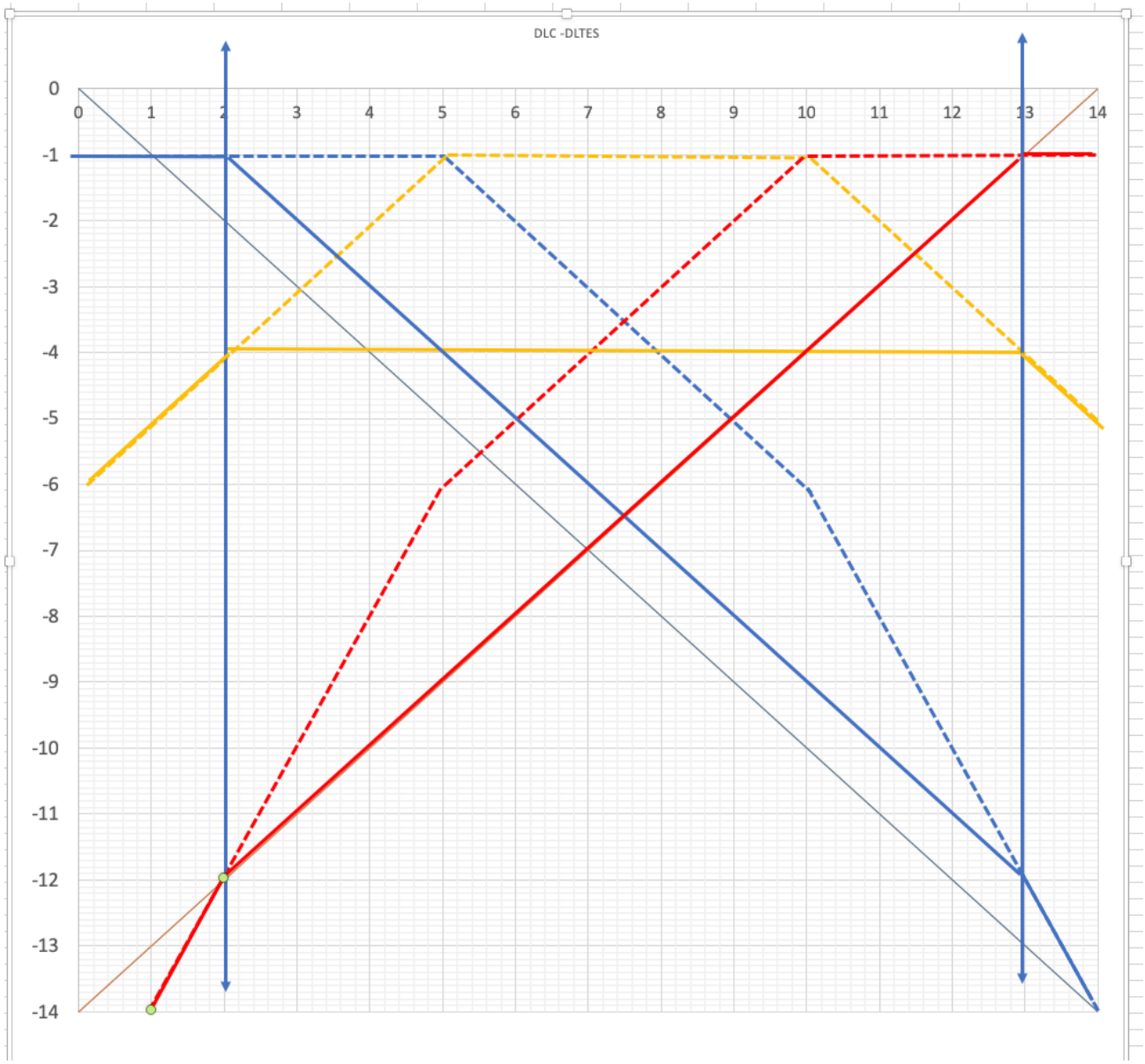
DLC → DLTED

$\log[H_2Ox^+]$



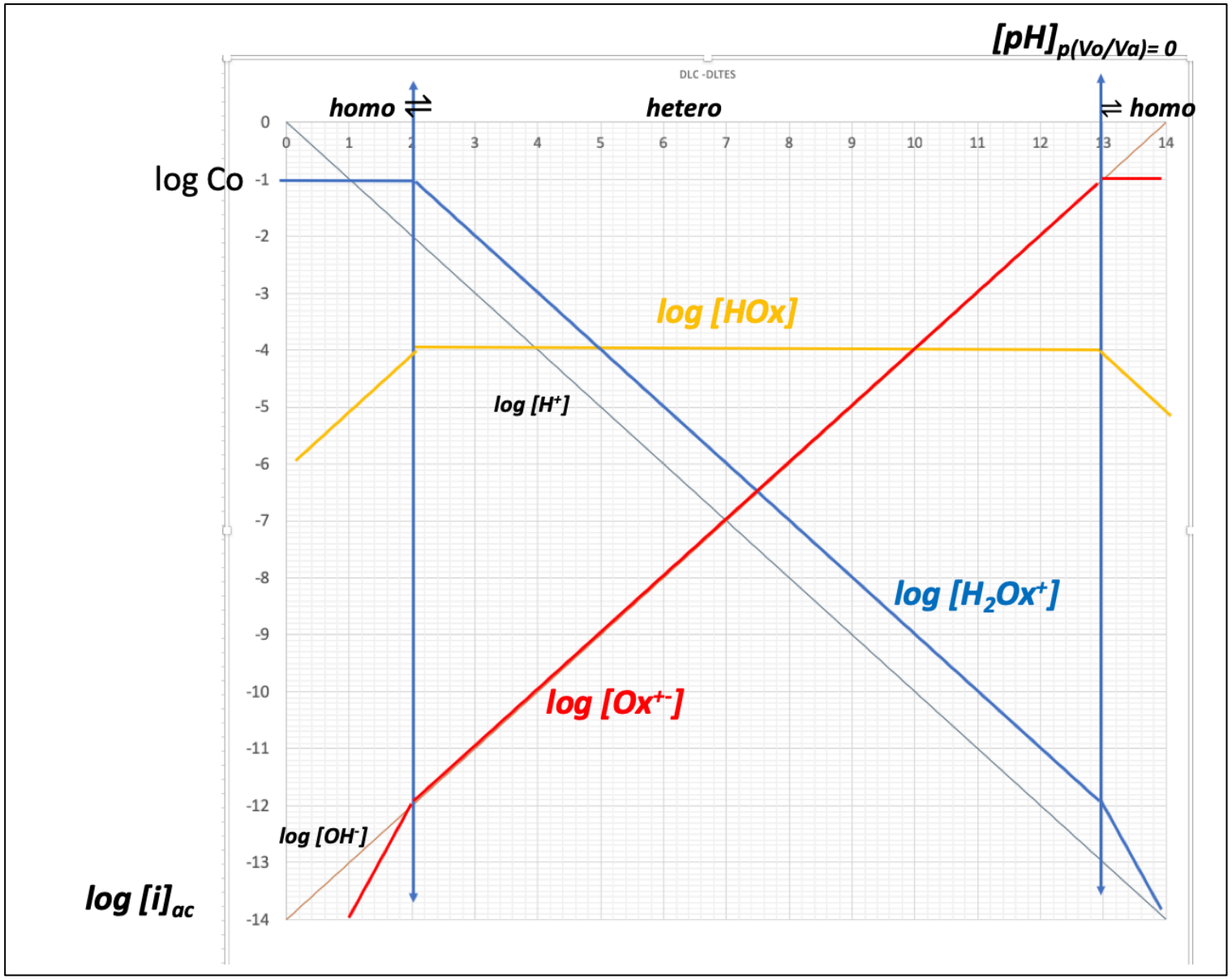
DLC → DLTED

$log\ [Ox^{-}]$



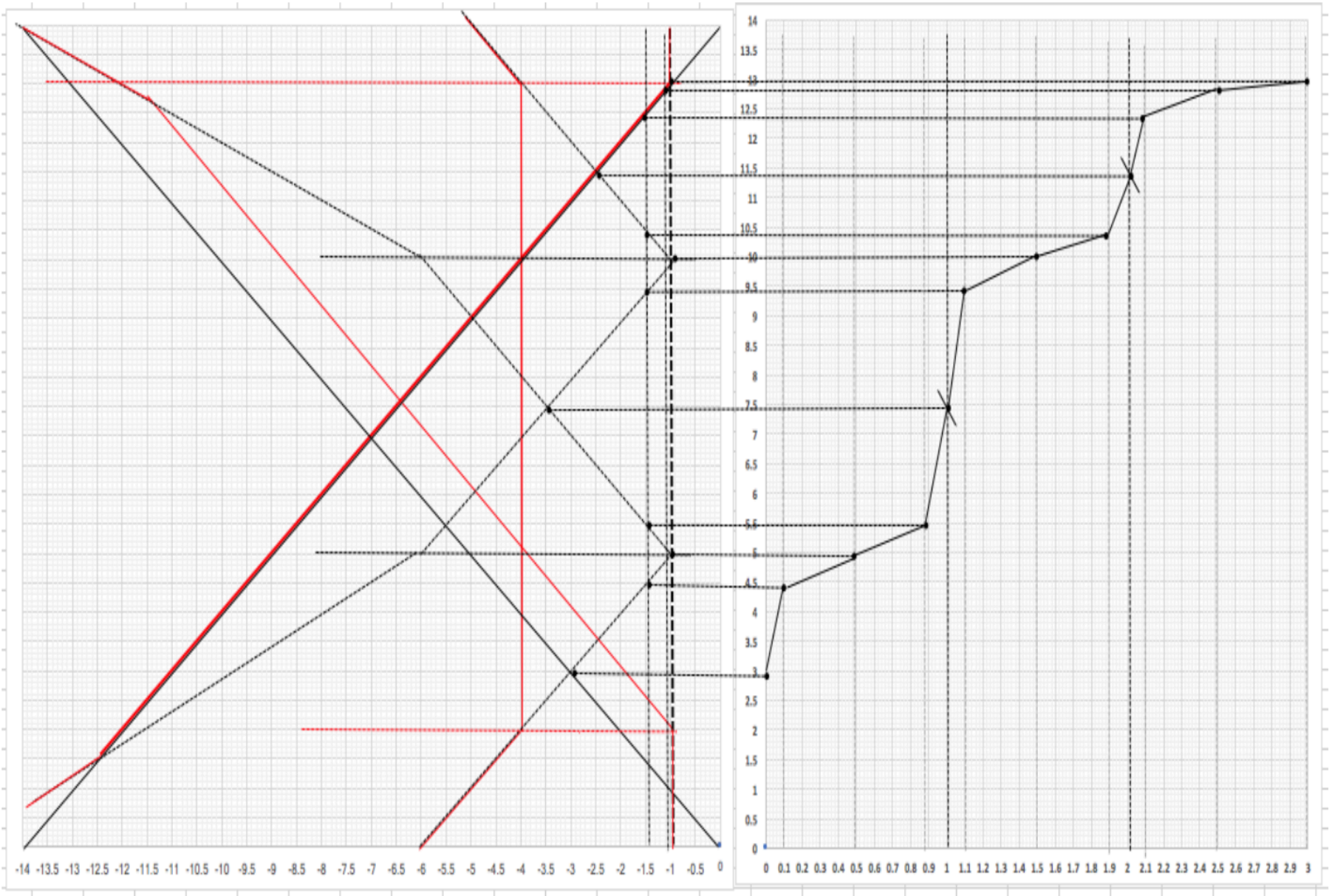
DLTED

p(Vo/Va) = 0



DLC

$F_{H_2OXCl} = Co$



DLTED
p(Vo/Va)= 0