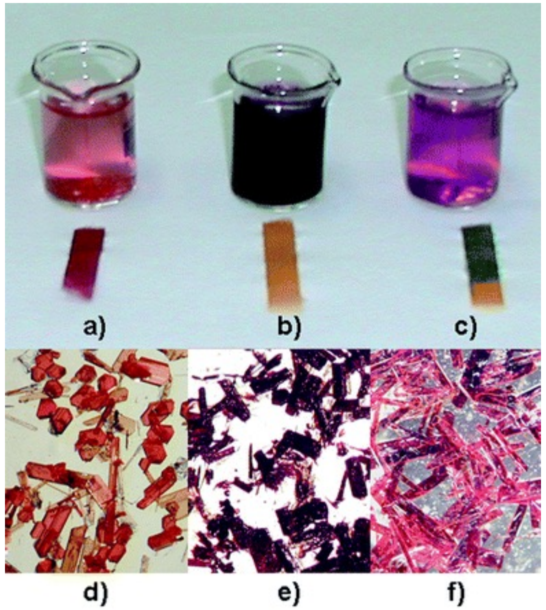
QA II
FQ- UNAM
Prof. Alejandro Baeza

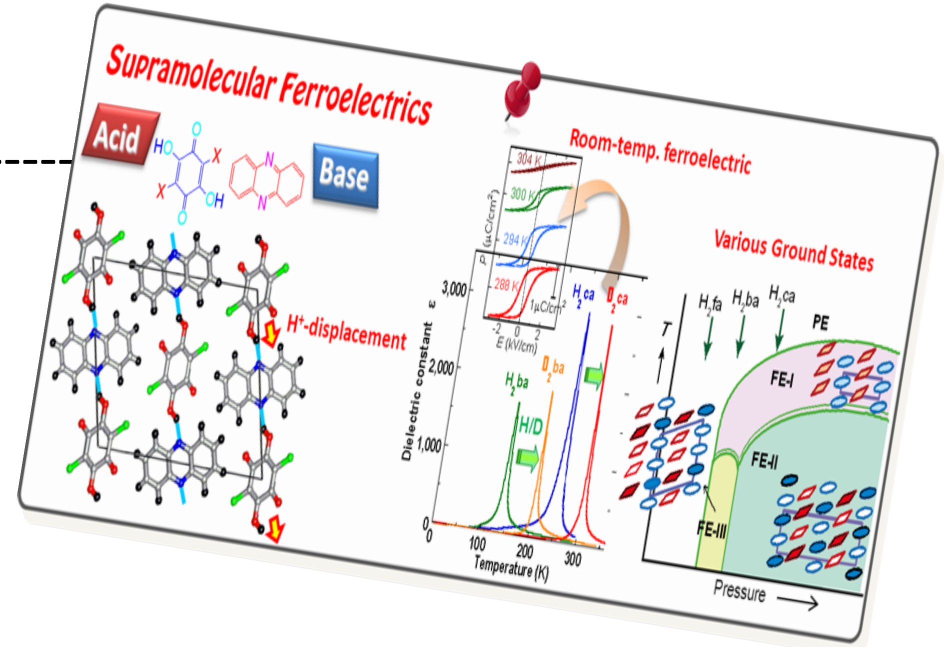
http://microelectrochemalexbaeza.com

Diagrama Lotaritmico de Transición de Estado de Solubilidad

DLTES



---------- **Cloranilato de Ca** ----------



El ácido cloranílico es un compuesto que puede formar complejos orgánicos con propiedades electricas buscadas como sustituto de componentes electrónicos metálicos , sus propiedades dependen de su comportamiento ácido base–solubilidad.

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TTF derivative of 2,5-aromatic disubstituted pyrrole, synthesis and electronic study

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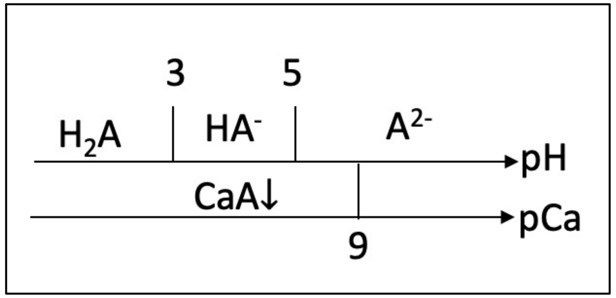
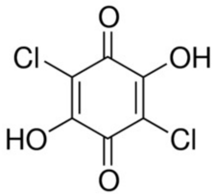
1. Introduction

The study of electronic materials has been growing and opening new important areas [1–3], the study of this kind of compounds takes account mainly on the energy of the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) levels and the orbital interactions. These last interactions are fundamental for the communication between two different pair of molecules that can show interesting electronic interchanges [4].

DUZP-DUPE combinados:



H_2A =



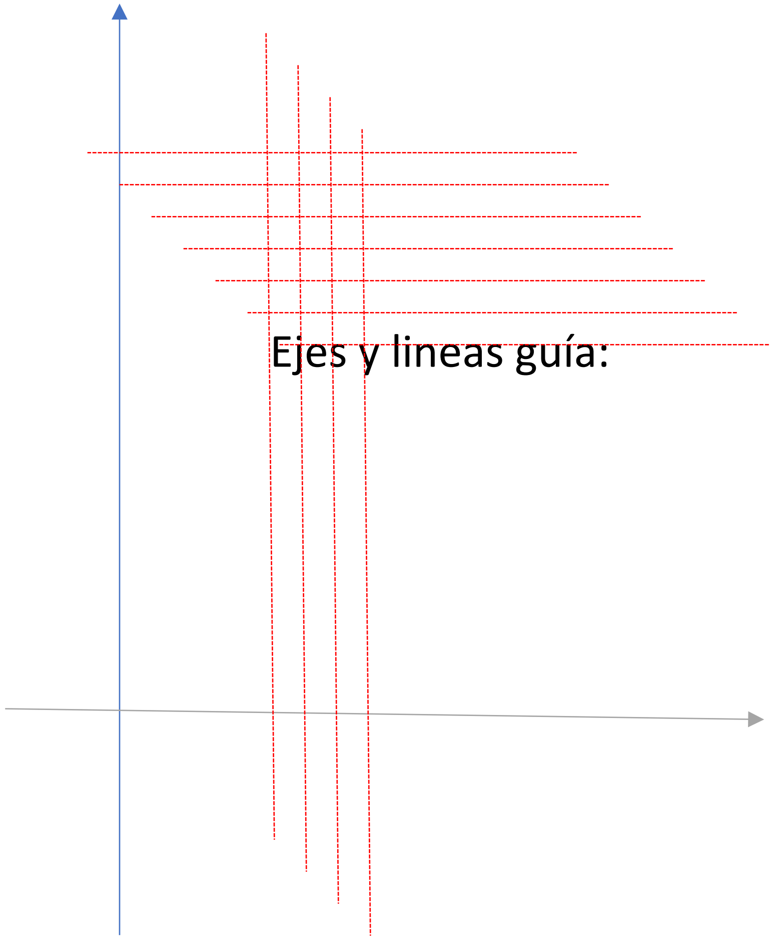
1º) DZPE, pH =f(pCa)

2º) DLTES, log [*S*] = f(pH)$_{pCa2}$

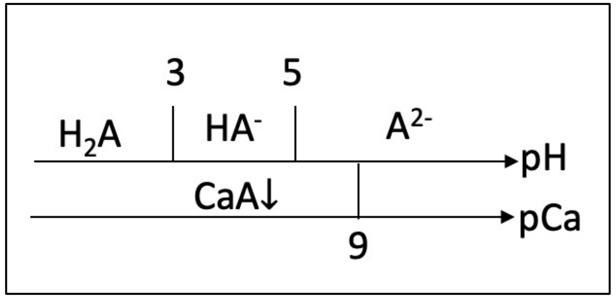
3º) DLTES=f(log[i])= f(*f*)

1º) DZPE, pH =f(pCa)

Ejes y lineas guía:



1º) DZPE, pH =f(pCa)



(a) $pH = pKa_1$

$HA^- \rightleftharpoons A^{2-} + H^+$

(b). $pH = pKa_2$

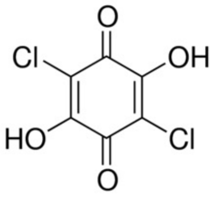
$H_2A \rightleftharpoons HA^- + H^+$

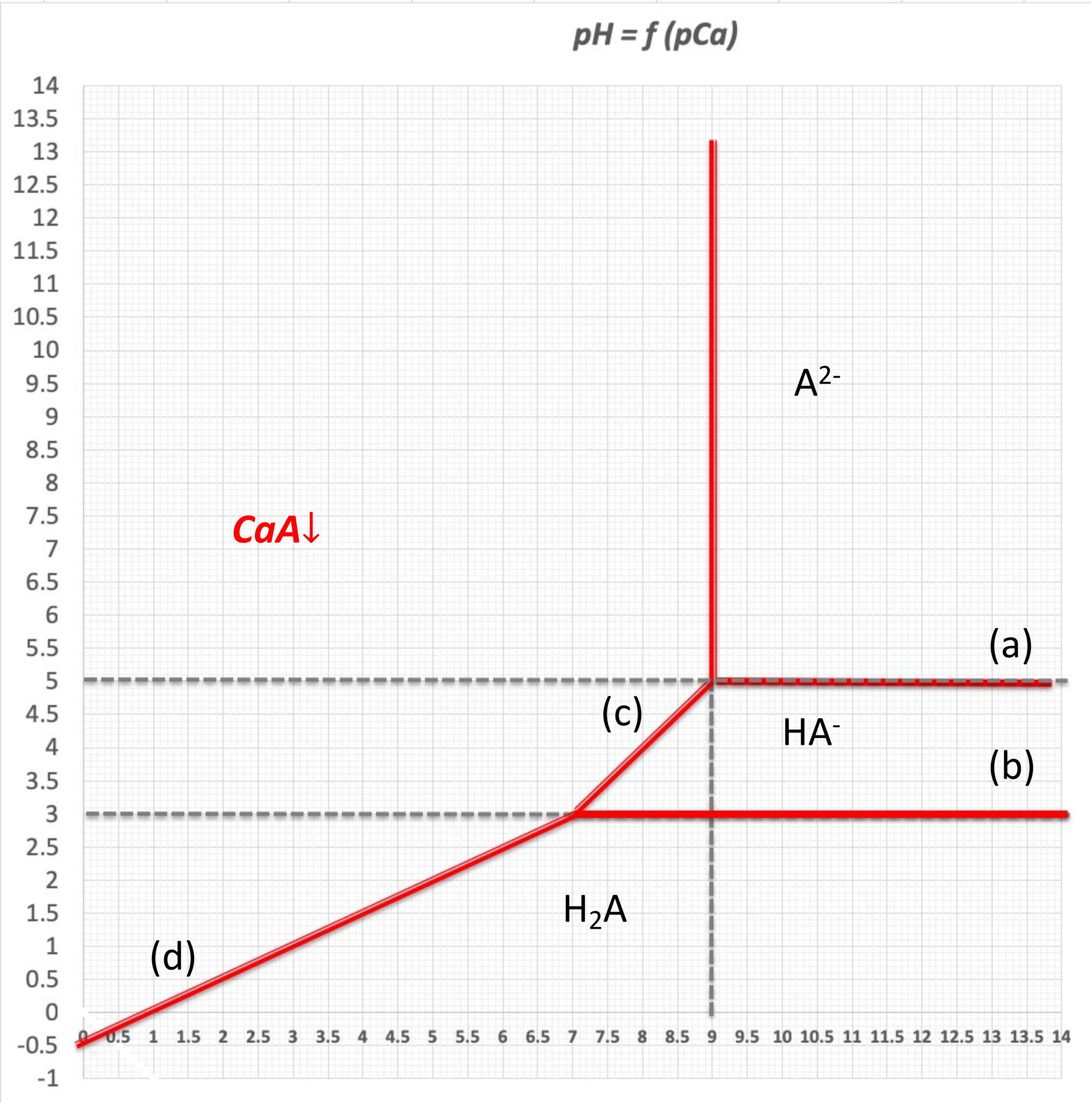
(C) $pH = pKa_1{}' = pKa_1 - pKs + pCa$

$HA^- + Ca^{2+} \rightleftharpoons CaA\downarrow + H^+$

(d) $2pH = pKa_{gbl}{}' = pKa_1 + pKa_2 - pKs + pCa$

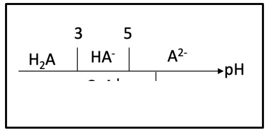
$H_2A + Ca^{2+} \rightleftharpoons CaA\downarrow + 2H^+$

H_2A = 



A pCa > pKs = 9: DLC HOMOGENEO

Trazo formal: funciones polinomiales:



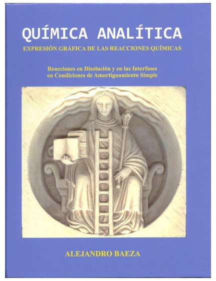
$$\log[i] = \log Co + log\Phi_i$$

$$\Phi_A = \left[1 + K_{HA}^{H}[H^+] + K_{H_2A}^{2H}[H^+]^2\right]^{-1}$$
$$\Phi_{HA} = \Phi_A\left(K_{HA}^{H}[H^+]\right)$$
$$\Phi_{H_2A} = \Phi_A\left(K_{H_2A}^{2H}[H^+]^2\right)$$

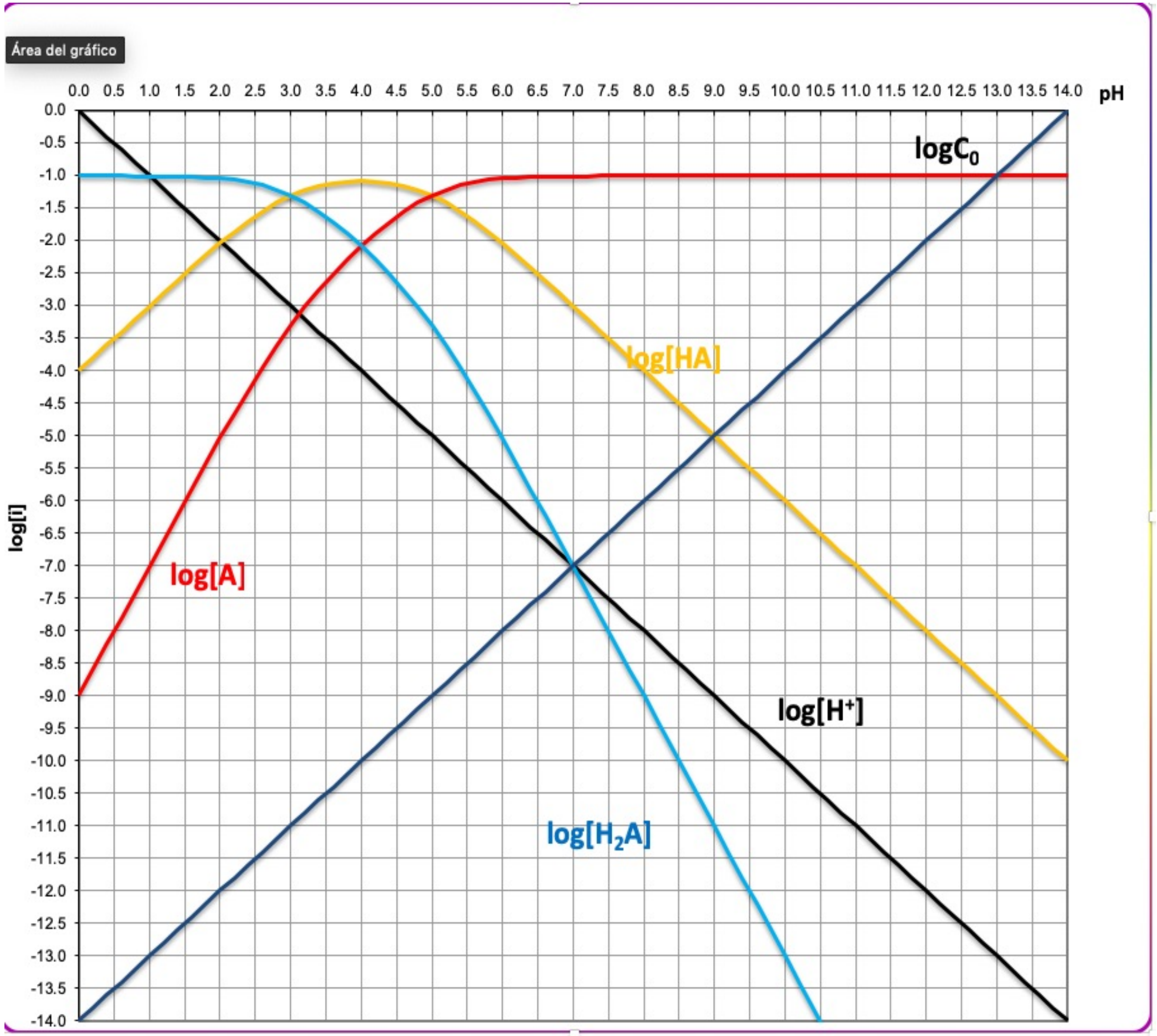
$\log[A^{2-}]$ = log Co + log Φ_A – $\log[1 + K_{HA}^{H}[H^+] + K_{H_2A}^{2H}[H^+]^2]$

$\log[HA^-]$ = log Co + log Φ_{HA} = log Co + log Φ_A + $log\left[K_{HA}^{H}[H^+]\right]$

$log[H_2A]$=log Co + log Φ_{H_2A} = log Co + log Φ_A + log $\left[K_{H_2A}^{2H}[H^+]^2\right]$

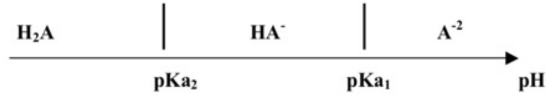


A. Baeza. Química Analítica. *Expresión Gráfica de las Reacciones Químicas*. S. y G. Ediciones. **2010**.
http://microelectrochemalexbaeza.com/wp-content/uploads/2015/06/BOOK-I-complete-REV-2010c2012_I.pdf

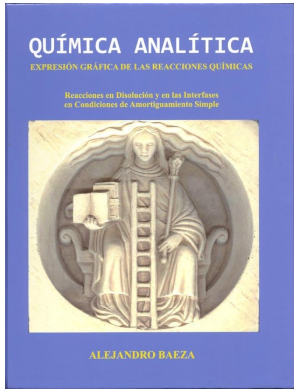


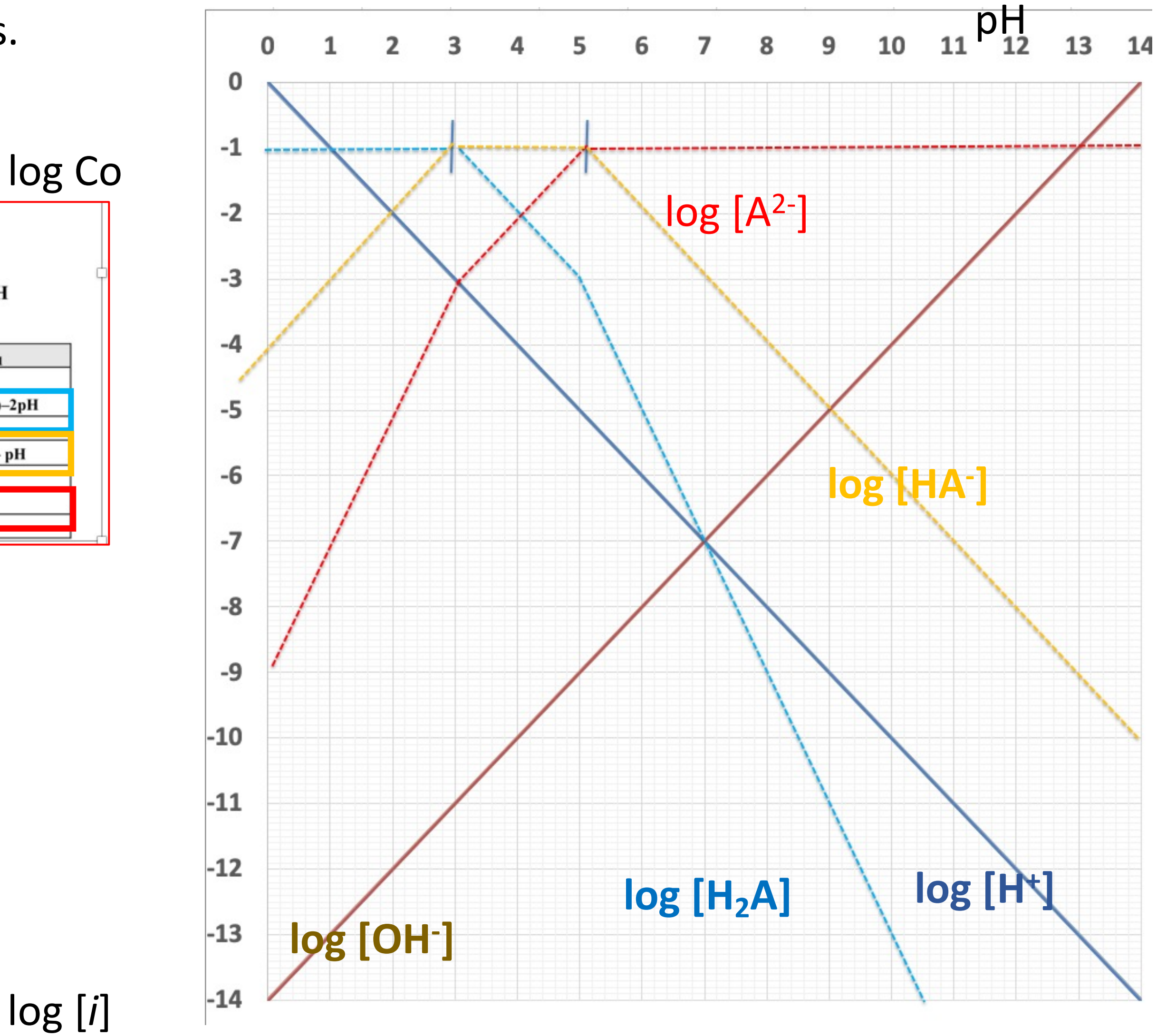
A pCa > pKs = 9: DLC HOMOGENEO

Trazo rápido: polinomios reducidos.



	pH << pKa$_2$:	pKa$_2$ <<pH << pKa$_1$	pH >> pKa$_1$
log [H$_2$A]	(1) log Co,	(2) log Co +pKa$_2$ – pH	(3) log Co+(pKa$_1$+pKa$_2$)–2pH
log [HA$^-$]	(4) log Co –pKa$_2$ + pH	(5) log Co	(6) log Co +pKa$_1$ – pH
log [A^{2-}]	(7) log Co – (pKa$_1$+pKa$_2$) +2pH	(8) log Co –pKa$_1$ + pH	(9) log Co





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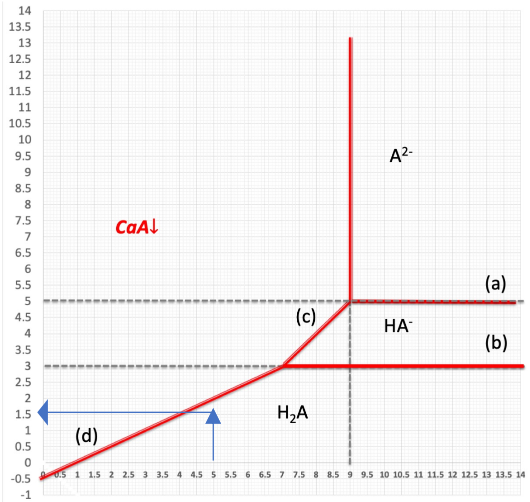
2º) DLTES, log [S] = f(pH)$_{pCa=5}$

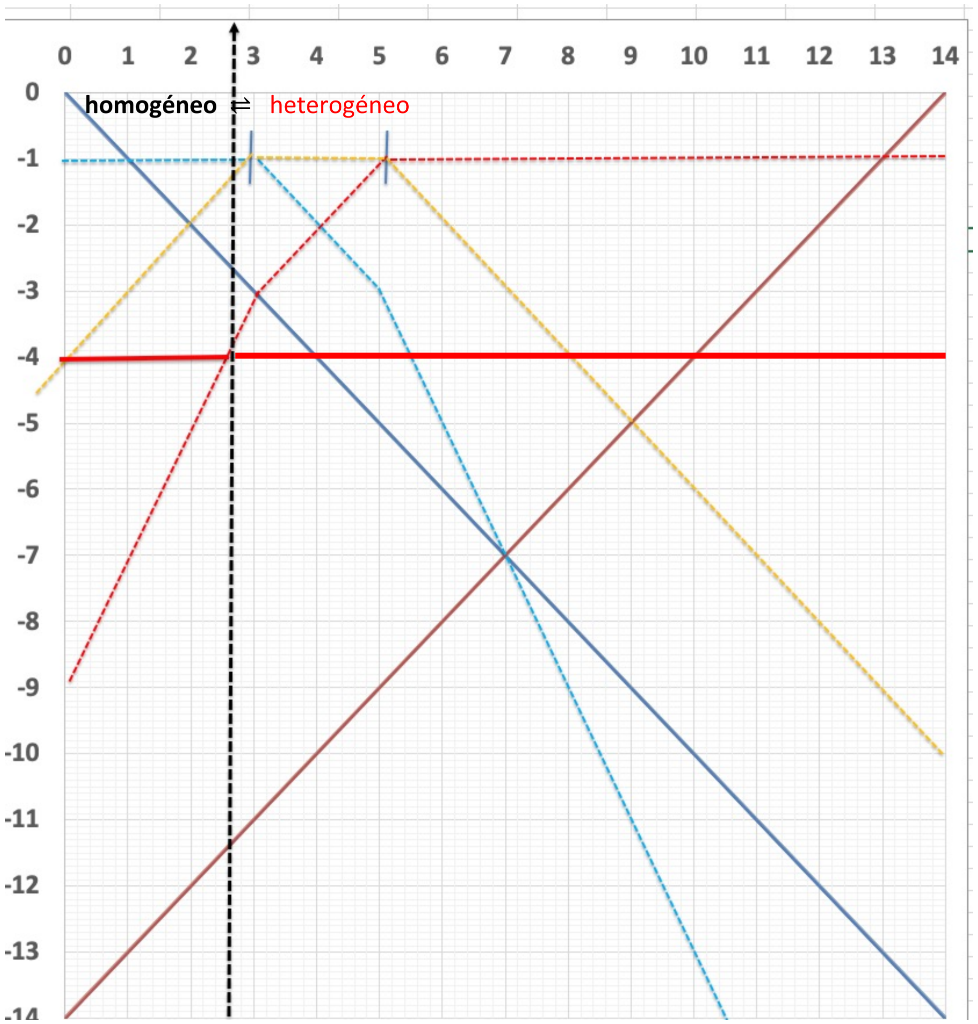


A pCa = 5: $Ks = [A^{2-}][Ca^{2+}]$

$Ks = 10^{-9} = [A^{2-}]10^{-5}$

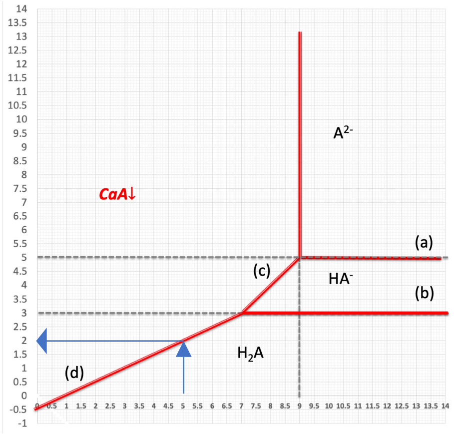
$\log [A^{2-}] = -4 = \log S'$

A partir del DLC homogeneo
Se determina el pH de inicio
De precipitación: cambio de estado:



Se determinan log $[A^{2-}]$ definitivos en ambos estados: ⟹

2º) DLTES, log [S] = f(pH)$_{pCa=5}$



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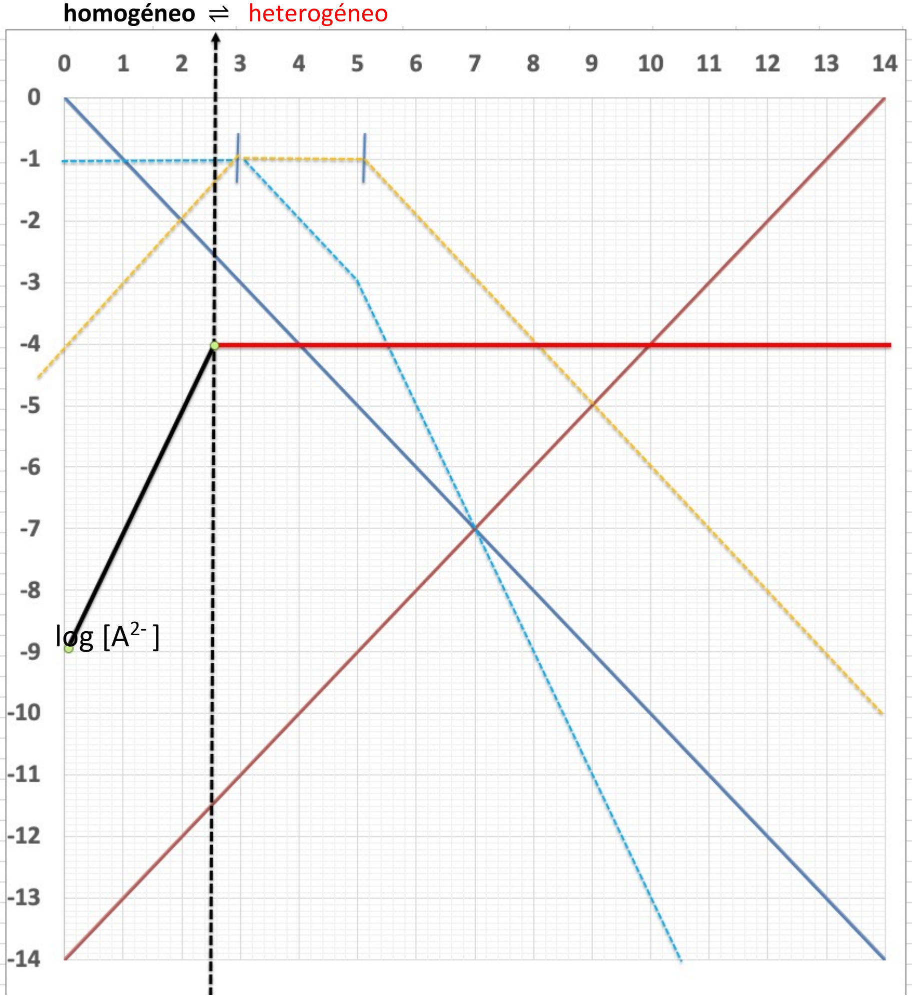

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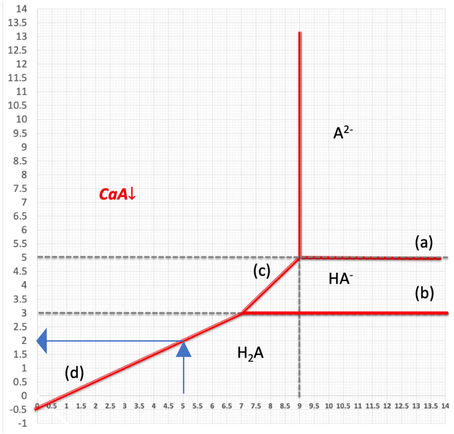

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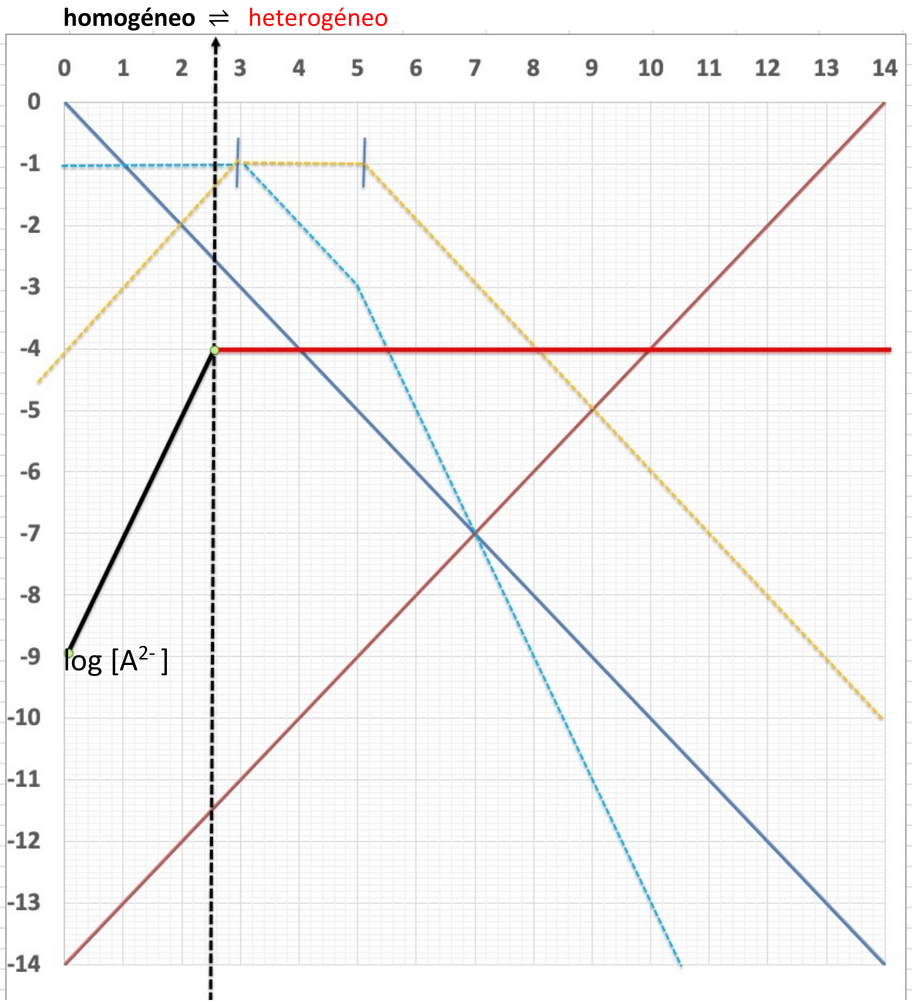
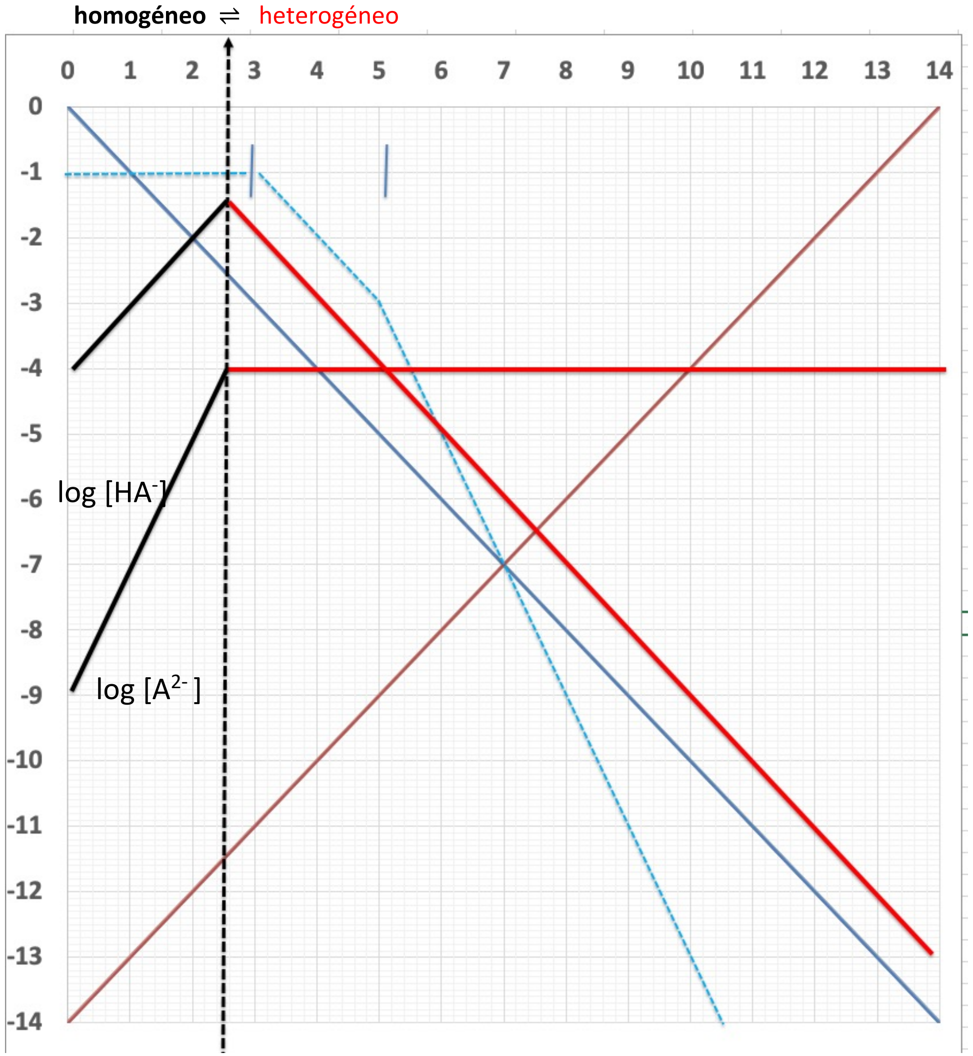


2º) DLTES, log [*S*] = f(pH)$_{pCa=5}$

Determinado el pH de transición de estado
Se busca log [HA$^-$] en medio heterogeneo según:

$HA^- + Ca^{2+} \rightleftharpoons CaA\downarrow + H^+$
log S´= pK_{gbl} + pCa –pH, ergo:

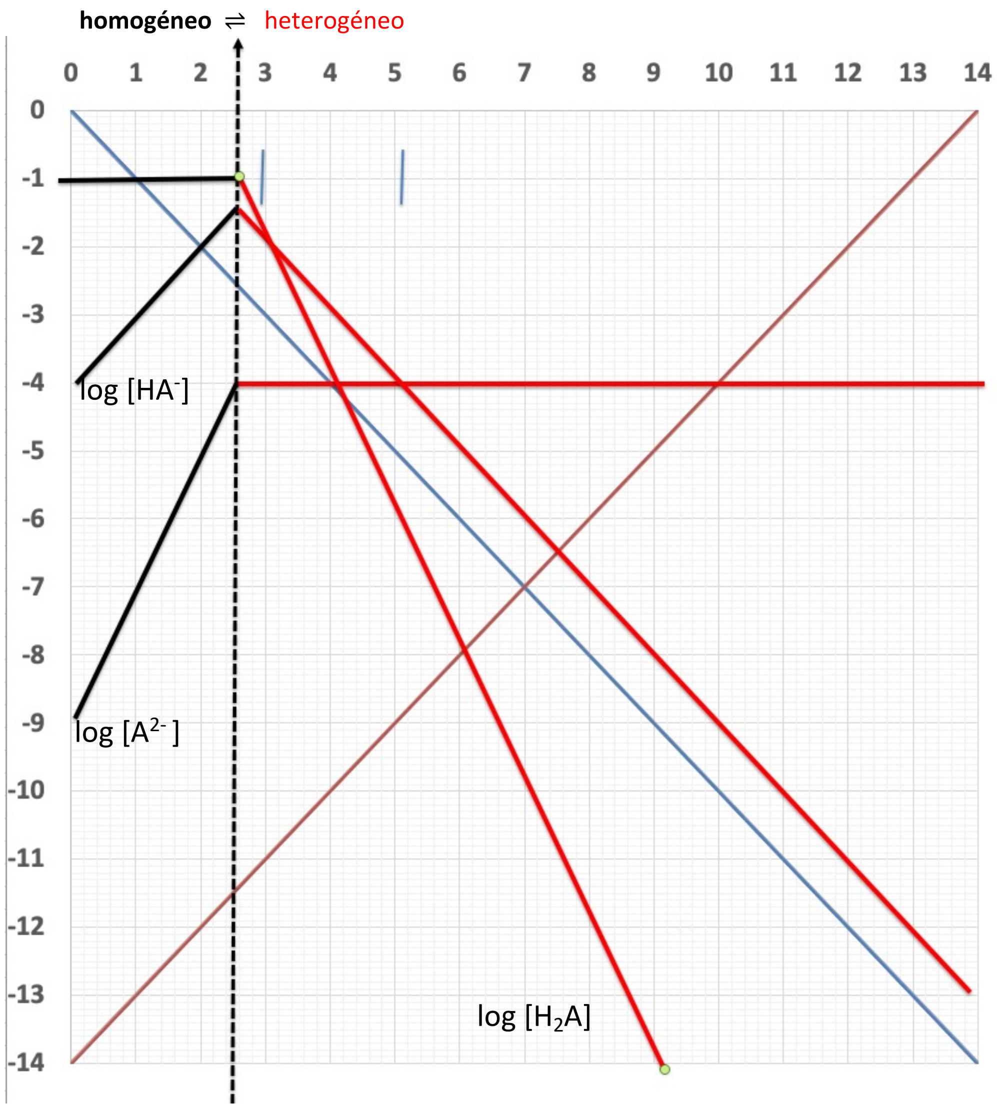
Desaparecen log [HA$^-$] en medio homogeneo:



Determinado el pH de transición de estado
Se busca log [H_2A] en medio heterogeneo según:

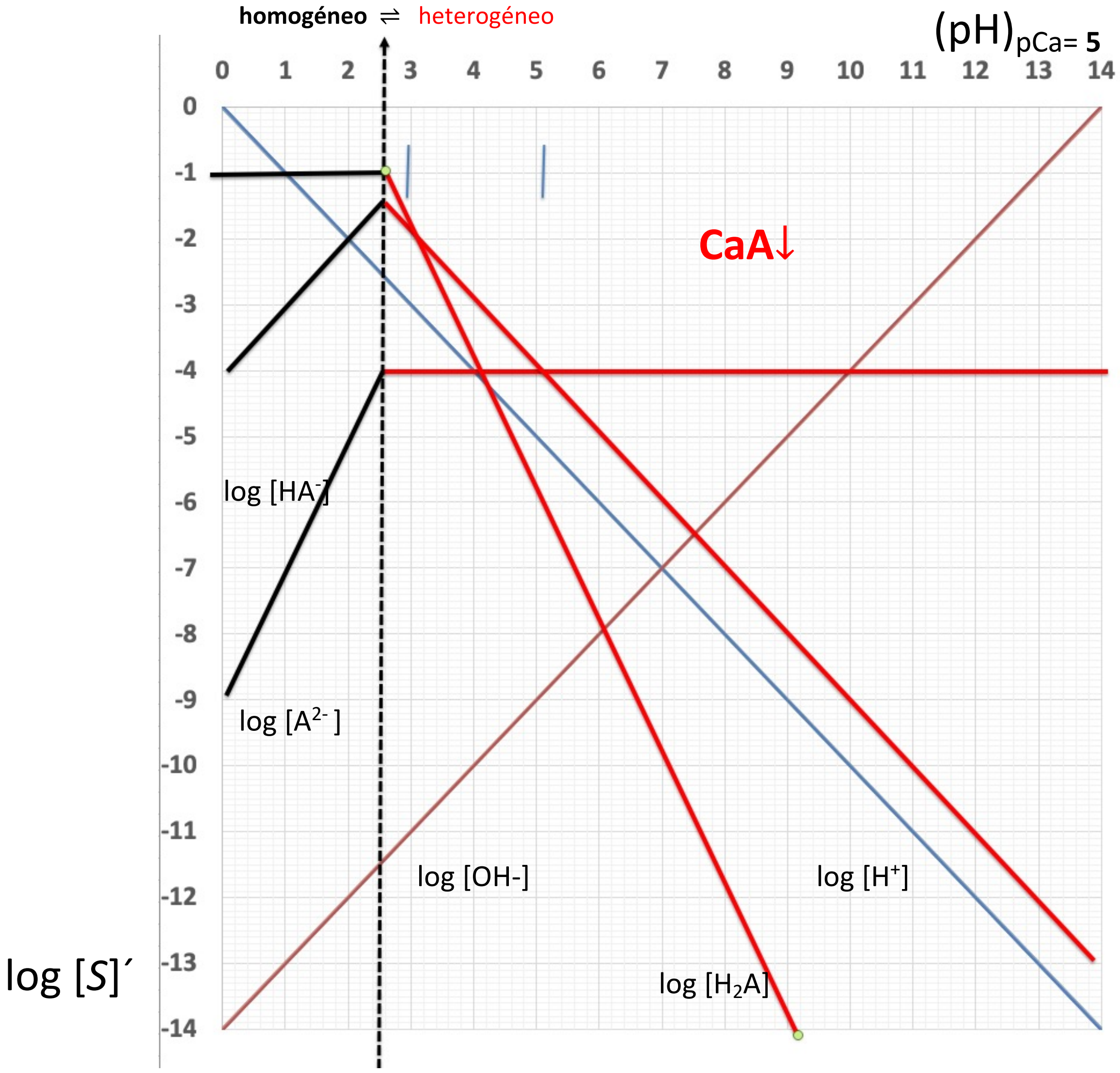
$H_2A + Ca^{2+} \rightleftharpoons CaA\downarrow + 2H^+$
log S´= pK_{gbl} + pCa –2pH, ergo:

Desaparecen log [H_2A] en medio homogeneo:



2º) DLTES, log [S] = f(pH)$_{pCa=5}$

El DLTES definitivo a pCa =5 queda:



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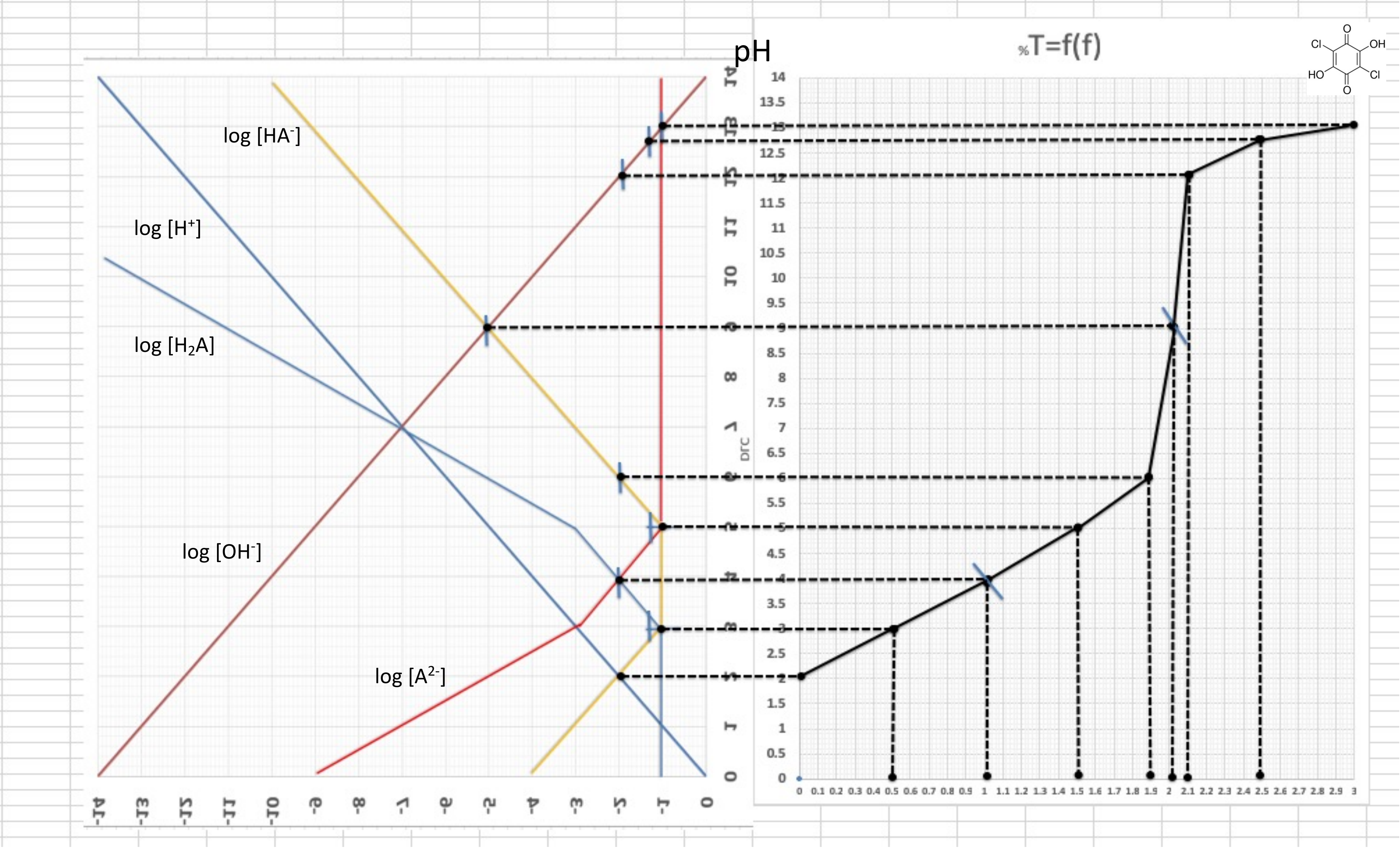

2º) DLTES, log [*S*] = $f(pH)_{pCa=5}$

3º) DLTES=f(log[i])= f(*f*)