Diagrama solubilidad

DLTES

QUÍMICA ANALÍTICA III
Sem. 2019-1

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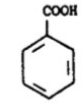
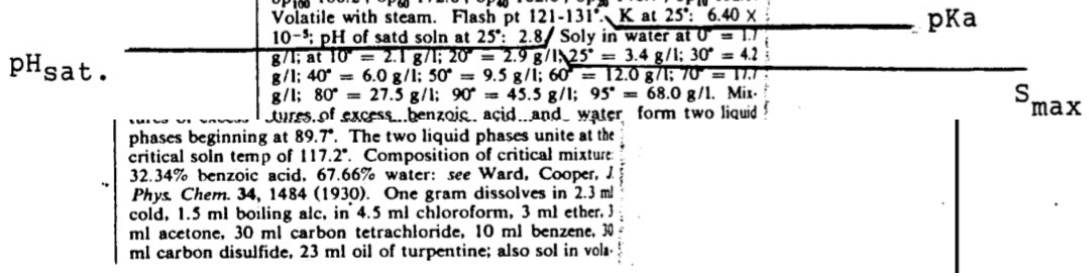
En la literatura química se encuentra la siguiente información sobre el ácido benzoico ("The Merck Index". An Encyclopedia of Chemicals and Drug. Ninth Edition. Pag. 142. Merck & Co., Inc. 1976):

1100. Benzoic Acid. Benzenecarboxylic acid; phenylformic acid; dracylic acid. $C_7H_6O_2$; mol wt 122.12. C 68.84%, H 4.95%, O 26.20%. Occurs in nature in free and combined forms. Gum benzoin may contain as much as 20%. Most berries contain appreciable amounts (around 0.05%). Excreted mainly as hippuric acid by almost all vertebrates, except fowl. The manuf of benzoic acid is discussed in Kirk-Othmer's *Encyclopedia of Chemical Technology*, **vol. 3** (Interscience, 2nd ed., 1964) pp 423-426. Processes described include the air oxidation of toluene, the hydrolysis of benzotrichloride, and the decarboxylaton of phthalic anhydride. Laboratory prepn from benzyl chloride: A. I. Vogel, *Practical Organic Chemistry* (Longmans, London, 3rd ed, 1959) p 755; from benzaldehyde: Gattermann-Wieland, *Praxis des organischen Chemikers* (de Gruyter, Berlin, 40th ed, 1961) p 193. Prepn of ultra-pure benzoic acid for use as titrimetric and calorimetric standard: Schwab, Wicher, *J. Res. Nat. Bur. Standards* **25**, 747 (1940).



Monoclinic tablets, plates, leaflets. Perfect 001 cleavage. d 1.321 (also reported as 1.266). mp 122.4°. Begins to sublime at around 100°. bp_{760} 249.2°; bp_{400} 227°; bp_{200} 205.8°; bp_{100} 186.2°; bp_{60} 172.8°; bp_{40} 162.6°; bp_{20} 146.7°; bp_{10} 132.1°. Volatile with steam. Flash pt 121-131°. K at 25°: 6.40 x 10^{-5}; pH of satd soln at 25°: 2.8. Soly in water at 0° = 1.7 g/l; at 10° = 2.1 g/l; 20° = 2.9 g/l; 25° = 3.4 g/l; 30° = 4.2 g/l; 40° = 6.0 g/l; 50° = 9.5 g/l; 60° = 12.0 g/l; 70° = 17.7 g/l; 80° = 27.5 g/l; 90° = 45.5 g/l; 95° = 68.0 g/l. Mixtures of excess benzoic acid and water form two liquid phases beginning at 89.7°. The two liquid phases unite at the critical soln temp of 117.2°. Composition of critical mixture: 32.34% benzoic acid, 67.66% water: *see* Ward, Cooper, *J. Phys. Chem.* **34**, 1484 (1930). One gram dissolves in 2.3 ml cold, 1.5 ml boiling alc, in 4.5 ml chloroform, 3 ml ether, 3 ml acetone, 30 ml carbon tetrachloride, 10 ml benzene, 30 ml carbon disulfide, 23 ml oil of turpentine; also sol in vola-

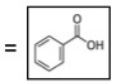


S_{max} = (3.4g/L) = 0.028mol/L

Log S_o = -1.6 ; pKa = 4.2

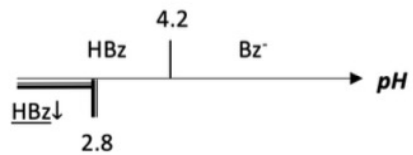
3.2.1 Solubilidad-acidez. Ejemplo (1). Diagrama logarítmico de transición de estado de solubilidad, DLTES, del ácido benzoico.

En la literatura se encuentran las propiedades fisicoquímicas del ácido benzoico ("The Merck Index", An enciclopedia of chemicasl and Drug, Ninth Edition. Pag. 142. Merck & Co., Inc, 2976):

HBz = 

MM = 122.12 g/mol
Ka = 6.4×10^{-5} M^2
$pH_{sat.}$ = 2.8
S_{max} = 3.4 g/L.

El ***DUPE*** correspondiente queda de la siguiente manera:



Las funciones logarítmicas en medio homogéneo y heterogéneo quedan en función de log S_0, log C_0, pKa, pKs:

En medio homogéneo:

$$log\ [HBz]\ =\ log\ Co\ -\ log[1 + 10^{-4.2+pH}]$$

$$log\ [Bz^{-}]\ =\ log\ Co\ -\ log[1 + 10^{4.2-pH}]$$

En medio heterogéneo:

$$log\ [HBz] = \log S_0 = \approx -1.6$$

$$\log\ S'\ = \log\ [HBz]' = \log S_0\ + \log[1 + 10^{-4.2+pH}]$$

La figura de la página siguiente muestra el ***DLTES*** del sistema del ácido benzoico para $\log C_0\ =\ -1$.

S_{max} = (3.4g/L) = 0.028mol/L

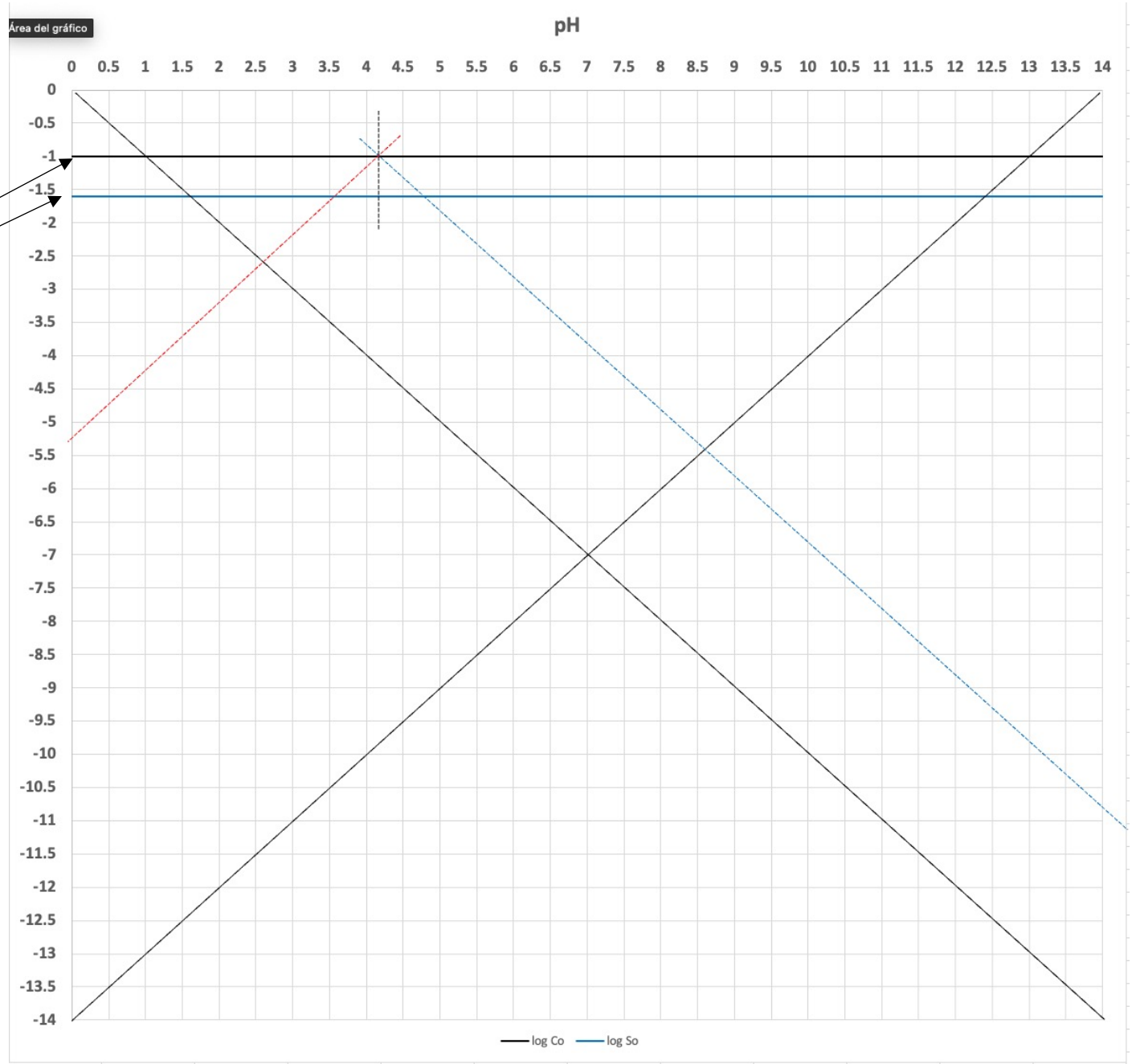
log (n_0/V_o) = log Co = -1

log S_o = -1.6

pKa = 4.2

log [HBz]

log [Bz^-]



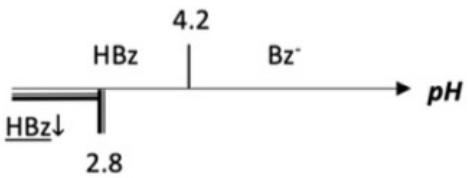
log Co

S_{max} = (3.4g/L) = 0.028mol/L

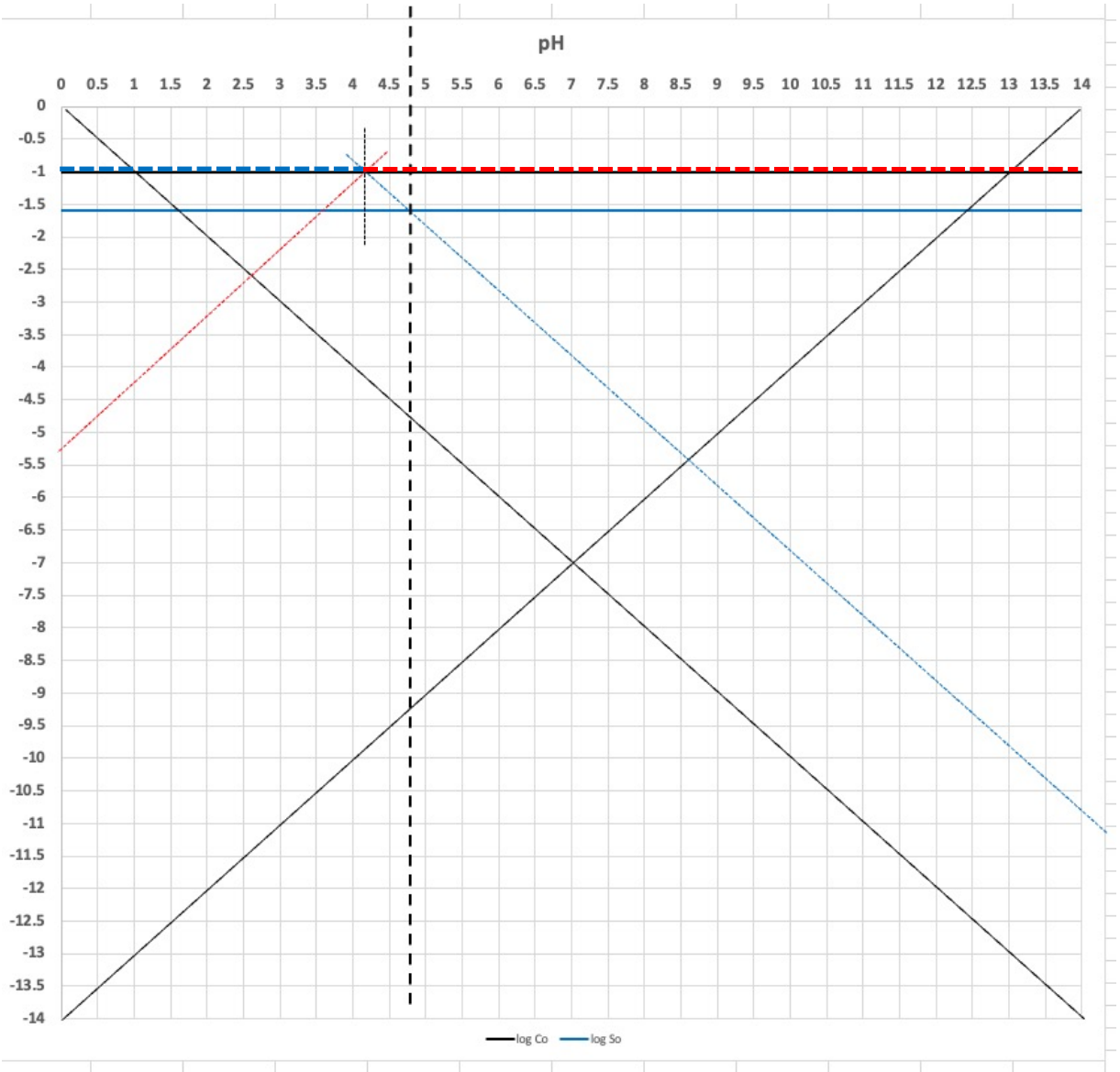
log (n_0/V_o) = log Co = -1

log S_o = -1.6

pKa = 4.2



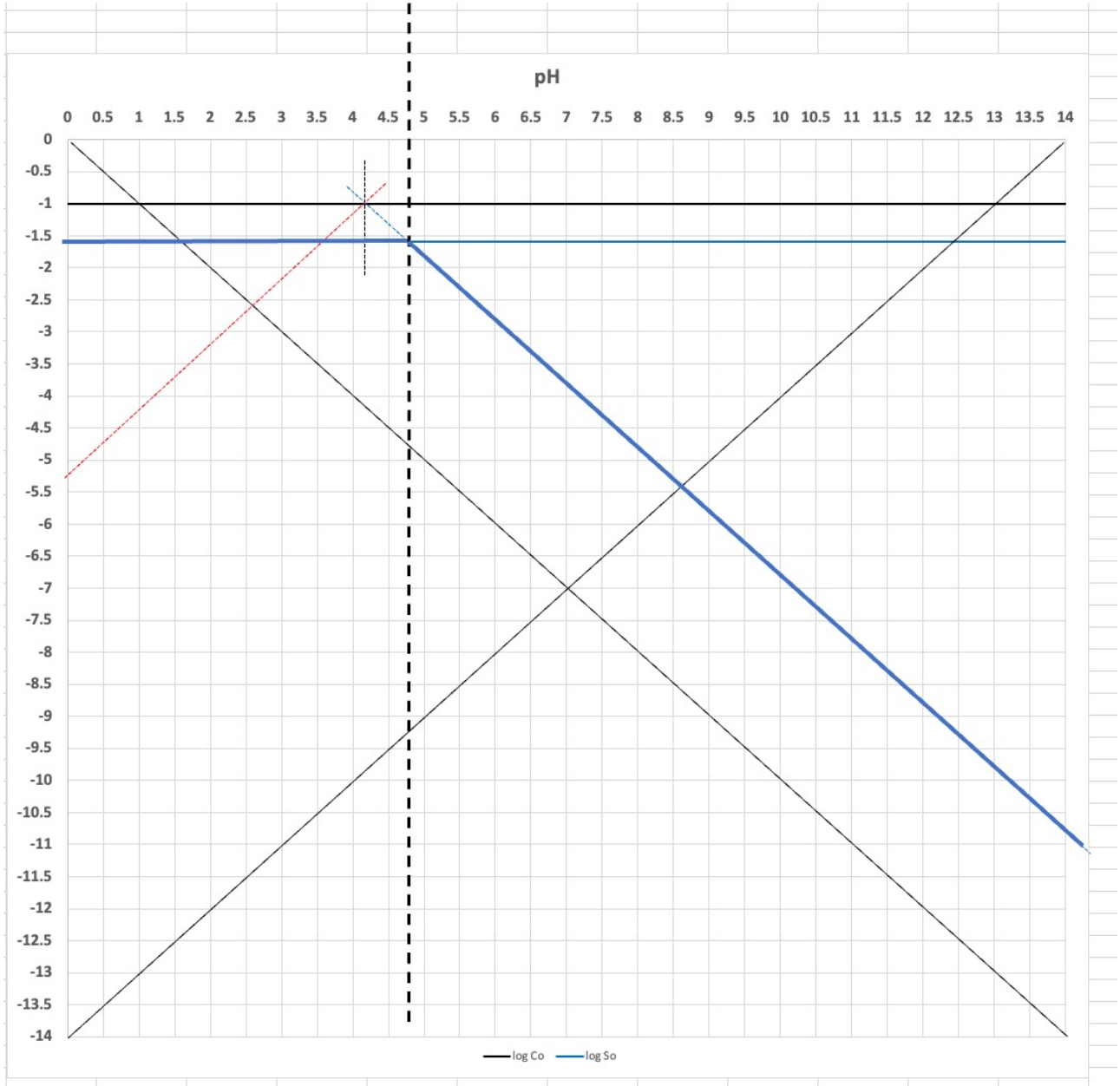
hetero ⇌ homo



log [HBz]

log [Bz^-]

log Co

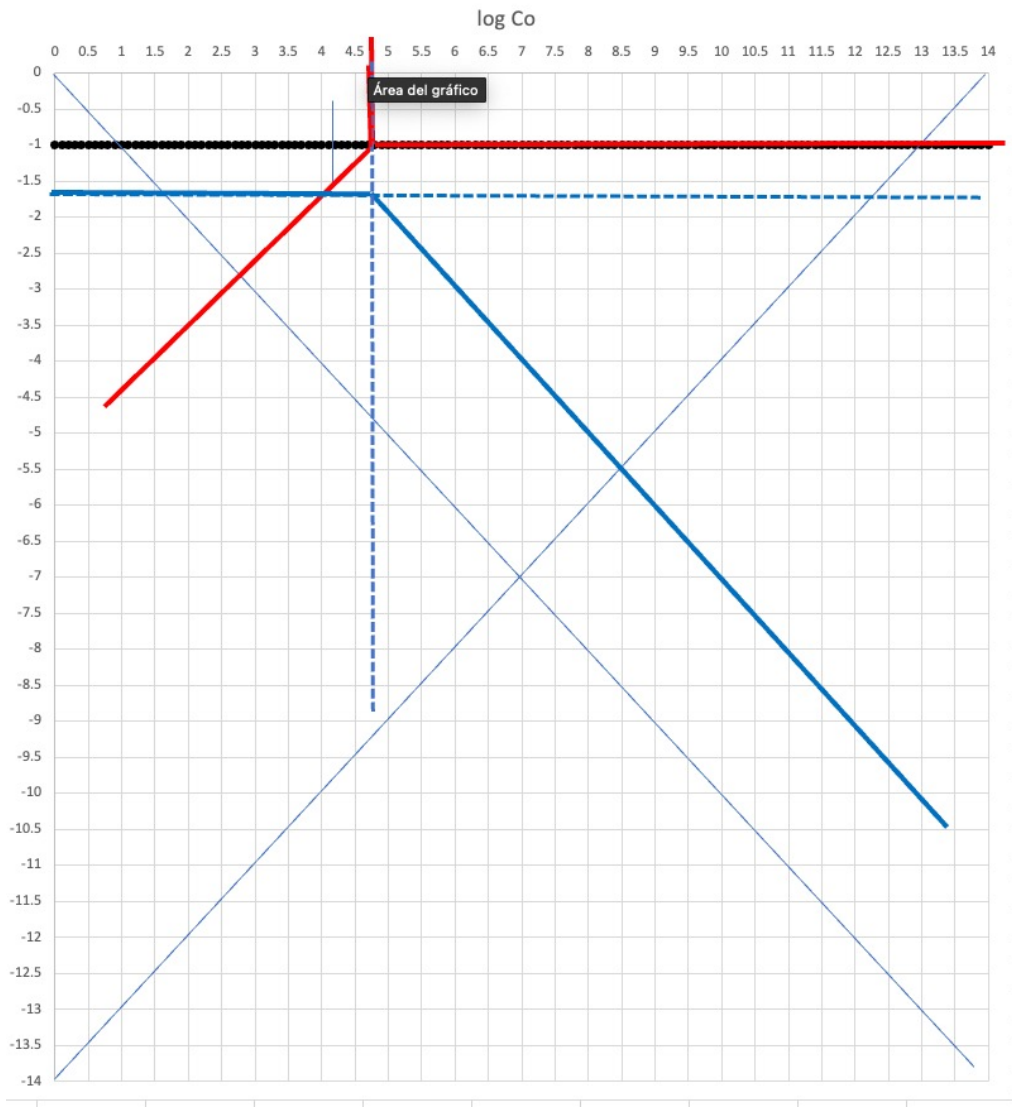


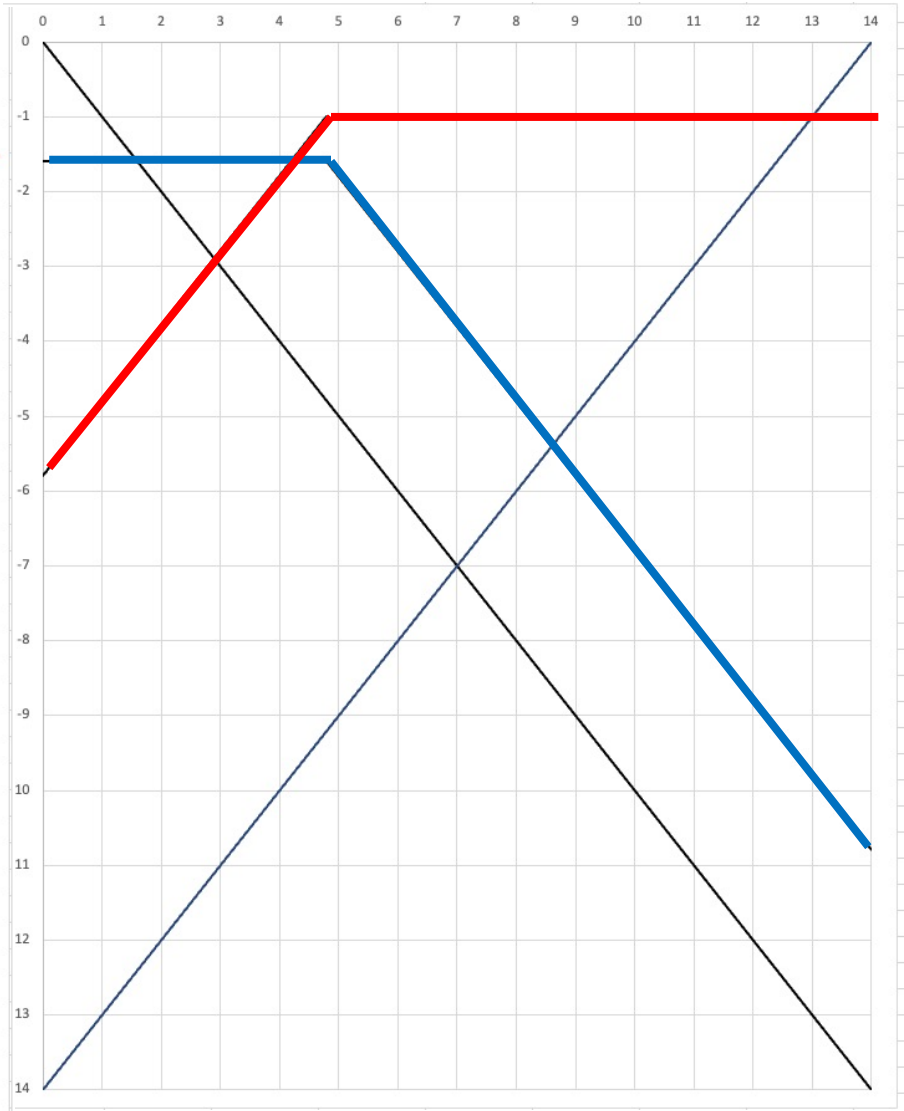
log [HBz]

log [Bz^-]

log [HBz]

log [Bz^-]





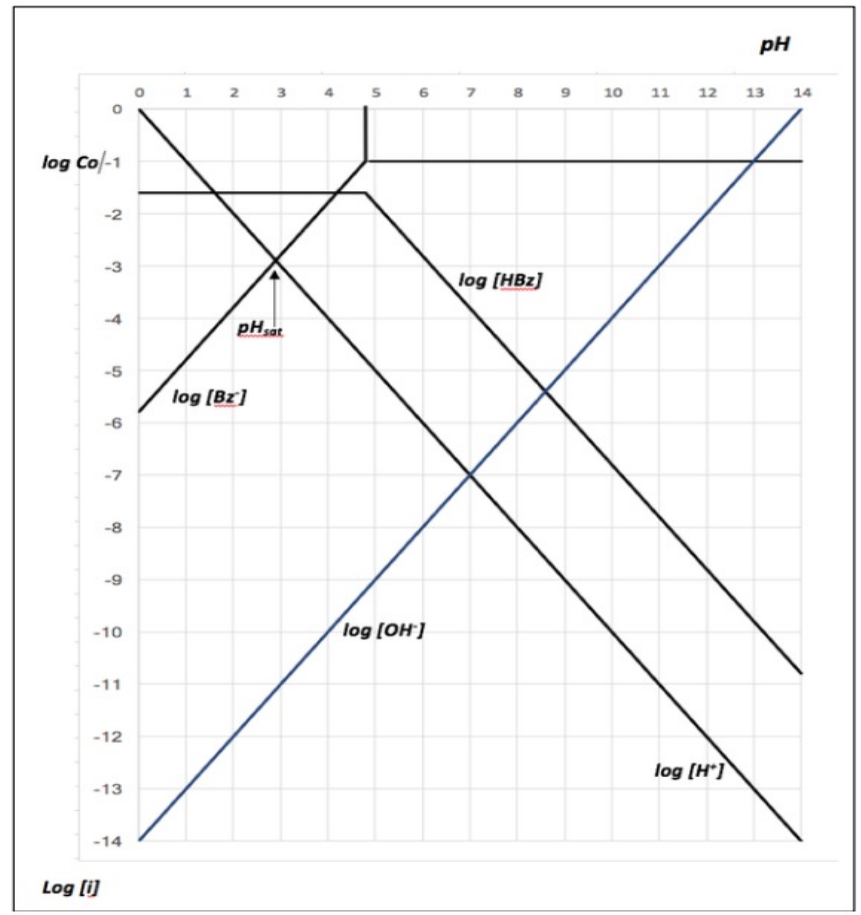
log [HBz]

log [Bz^-]

Del diagrama puede corroborarse el dato experimental del pH de saturación toda vez que se cumple:

$$\underline{HBz}\downarrow \rightleftarrows Bz^- + H^+$$

$\log [Bz^-] = \log [H^+] = -2.8$ y $\log [HBz] = -1.6$



DLTES del sistema del ácido benzoico para $\log C_0 = -1$.