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CEE 680: Water Chemistry

Lecture #11
Acids & Bases: Graphical Solutions I
(Stumm & Morgan, Chapt.3)
(Benjamin, Chapt. 4)

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Graphical Approach

- Independent Variable
 - pH: “the master variable”
- Two types of graphs
 - Distribution diagrams
 - alpha values, independent of concentration
 - Log concentration diagrams
 - pC-pH diagrams

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Monoprotic acids: calculations

Note: $\alpha_0 + \alpha_1 = 1$

- Start with C and K_a equations

$$C = [HA] + [A^-] \quad (3)$$

$$K_a = \frac{[H^+][A^-]}{[HA]} \quad (1)$$

$[A^-] = C - [HA]$ (1+3)
 $[HA] = C - [A^-]$ (1+3)

$$K_a = \frac{[H^+](C - [HA])}{[HA]}$$

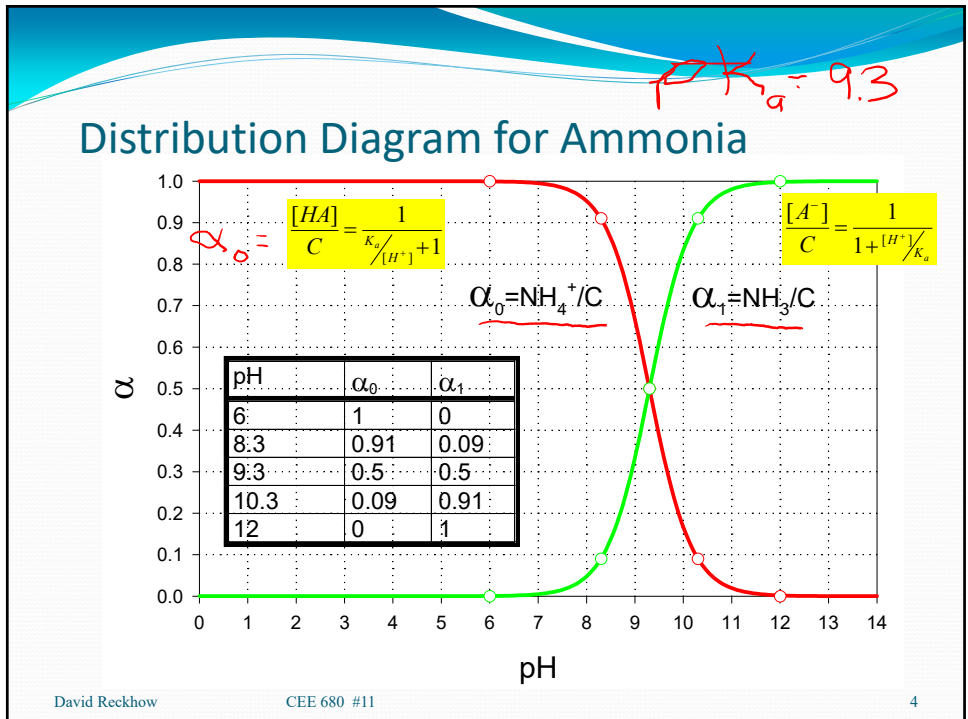
$$K_a[HA] = -[HA][H^+] + C[H^+]$$

$$K_a C - K_a[A^-] = [A^-][H^+]$$

For LogC vs pH diagrams: $[HA] = \frac{C[H^+]}{K_a + [H^+]}$ and $[A^-] = \frac{K_a C}{K_a + [H^+]}$

For distribution diagrams: $\alpha_0 = \frac{[HA]}{C} = \frac{1}{1 + [H^+]/K_a}$ and $\alpha_1 = \frac{[A^-]}{C} = \frac{1}{1 + K_a/[H^+]}$

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Preparing log C vs. pH Diagrams

- 1. Draw [H⁺] line
 - pH = -log[H⁺]
 - log[H⁺] = -pH ←
- 2. Draw [OH⁻] line
 - K_w=[H⁺][OH⁻] ②
 - log K_w= log[H⁺] + log[OH⁻]
 - log [OH⁻] = -log [H⁺] + log K_w
 - log [OH⁻] = pH - pK_w ←
- 3. Draw [HA] and [A⁻] lines
 - see next slide

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Calculations for log [HA] and log [A⁻] lines

$$[HA] = \frac{C[H^+]}{K_a + [H^+]}$$

$$[A^-] = \frac{K_a C}{K_a + [H^+]}$$

①+③

• If pH << pK_a, or [H⁺] >> K_a

Log [HA]=log C Log [A⁻]=log C + pH - pK_a

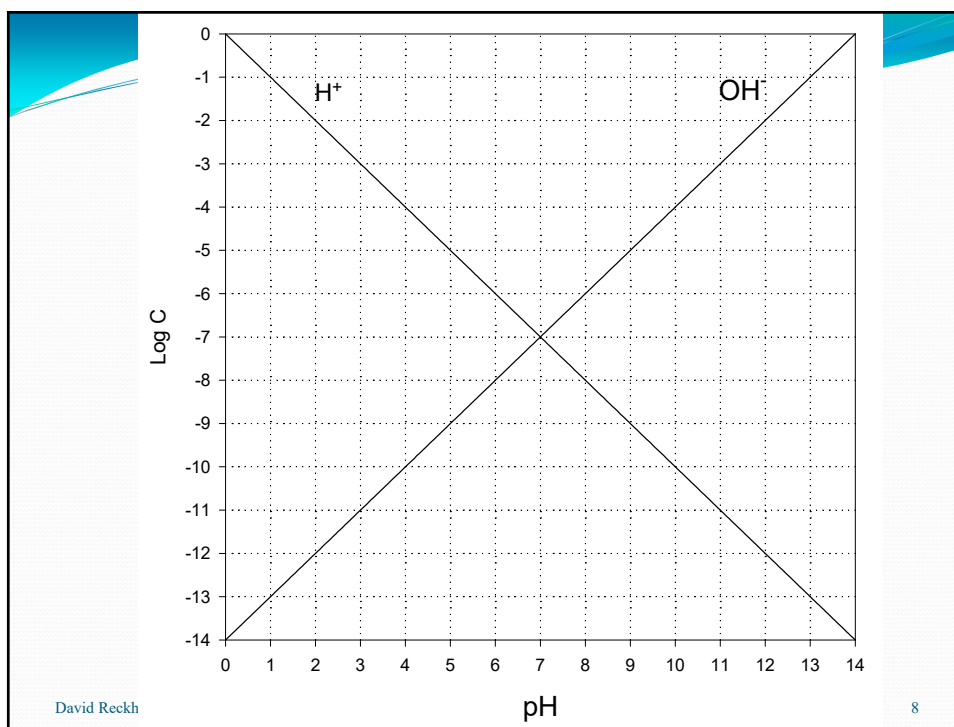
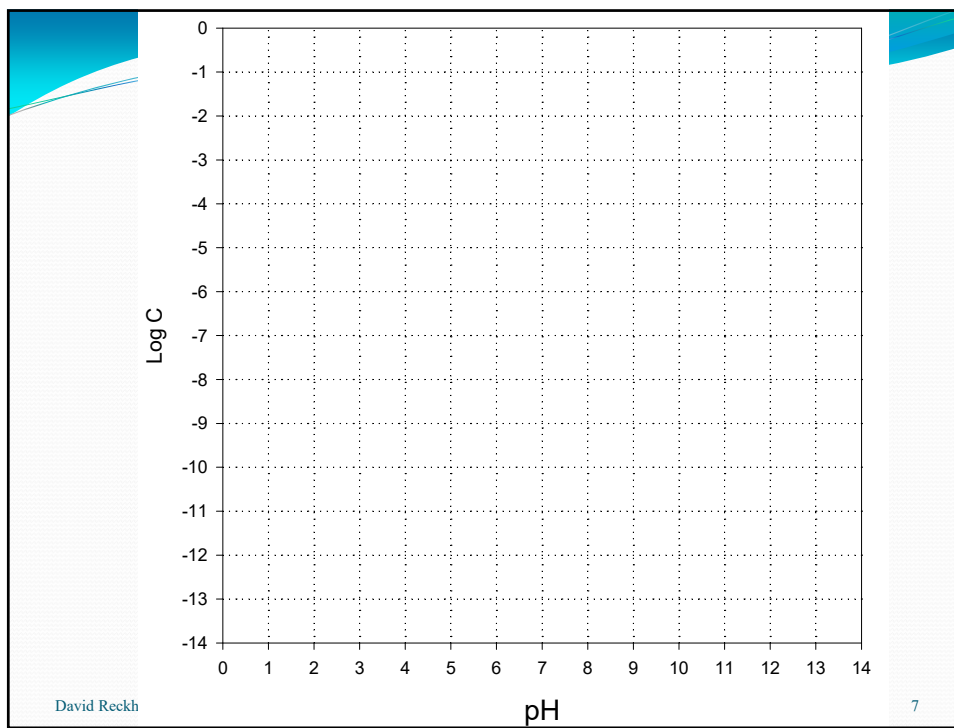
• If pH >> pK_a, or [H⁺] << K_a

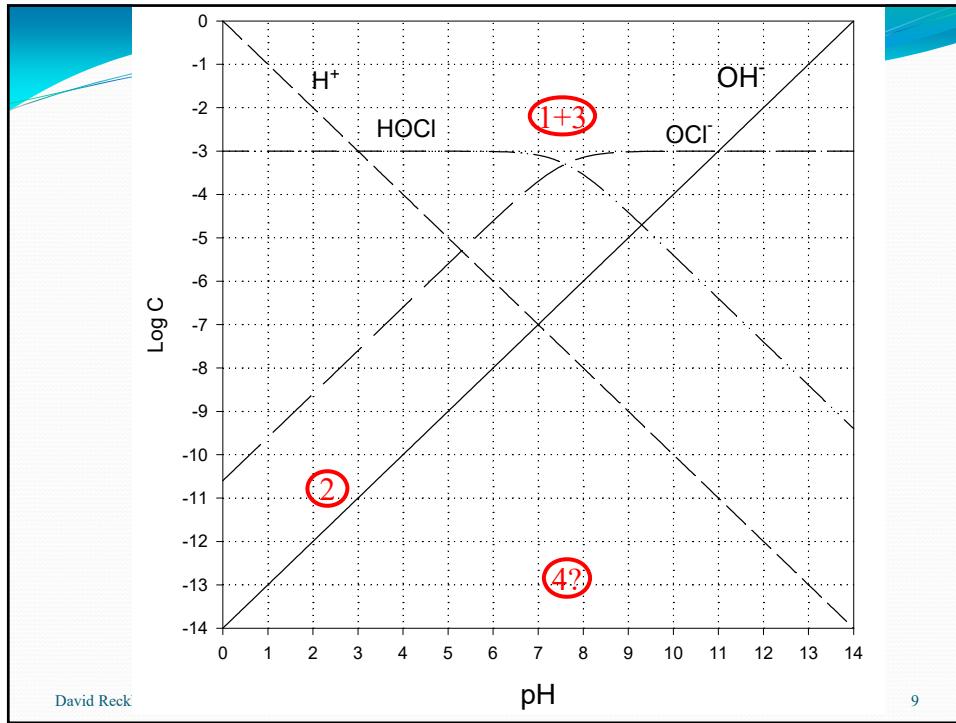
Log [HA]=log C - pH + pK_a Log [A⁻]=log C

• If pH = pK_a, or [H⁺] = K_a

Log [HA]=log C - 0.3 Log [A⁻]=log C - 0.3

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• To next lecture

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