Advanced Water Quality

Class 8: Acid Base Chemistry I

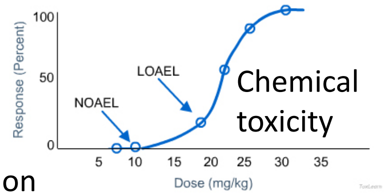
Today

- **Introduction**
- Basic concepts and terminology
- Acid and base strength
- Acid-base speciation vs. pH
- Introduction to solving simple acid speciation equilibrium problems

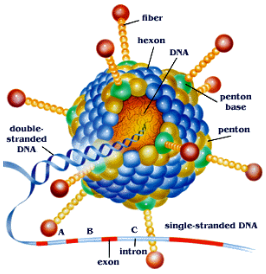
Introduction to Acid-Base Chemistry

- Acids/bases play important role in water quality
- Alter pH and affect many processes

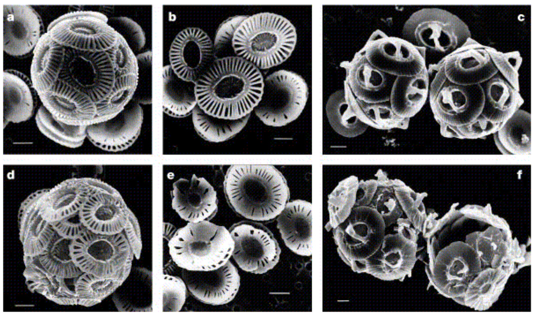
Dissolution/precipition



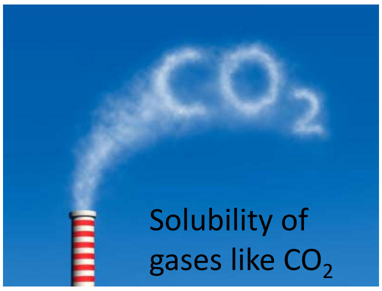
Chemical toxicity



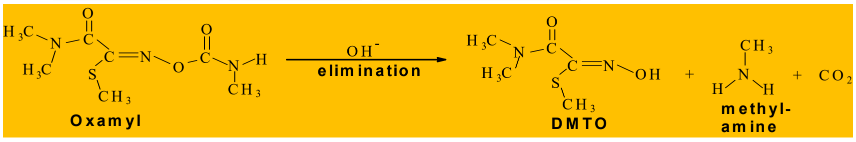
Potency of disinfectants



Catalyze chemical reactions



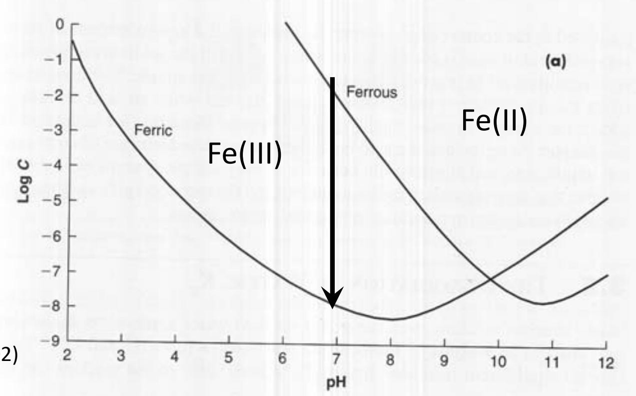
Solubility of gases like CO_2



Introduction to Acid-Base Chemistry

- Removal of dissolved iron from groundwater
  - Fe(II) & Fe(III) solubility highly pH dependent

Effect of pH on solubility of Fe(II) and Fe(III)



From Benjamin (2002)
Water Chemistry

- Dissolved Fe in groundwater typically Fe(II)

$$4\ Fe(II) + O_2 + 4\ H^+ \rightarrow Fe(III)\downarrow + 2\ H_2O$$

$$d[Fe(II)]/dt = -k[Fe(II)][O_2][OH^-]^2$$

Rate of Fe(II) oxidation increases 100-fold for each unit pH increase!!

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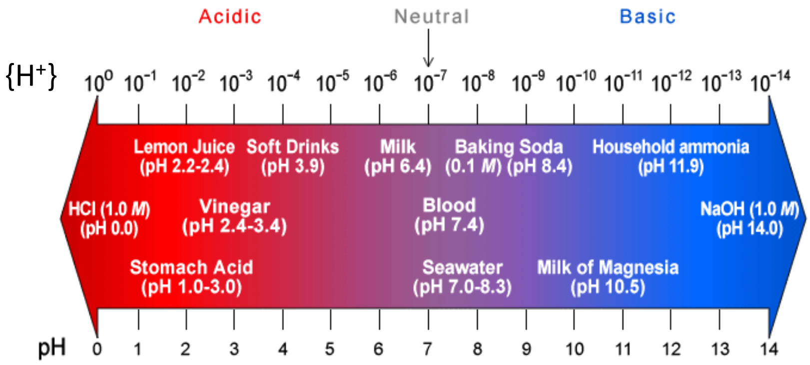
pH scale review

- pH = -log{H^+}
- pOH = -log{OH^-}



- Each unit change in scale = 10-fold change in {H^+} and {OH^-}
- What is neutral pH? *Solution where activity of H^+ and OH^- are equal*

Why is the pH scale 0 – 14?

$$H_2O \leftrightarrow H^+ + OH^-$$

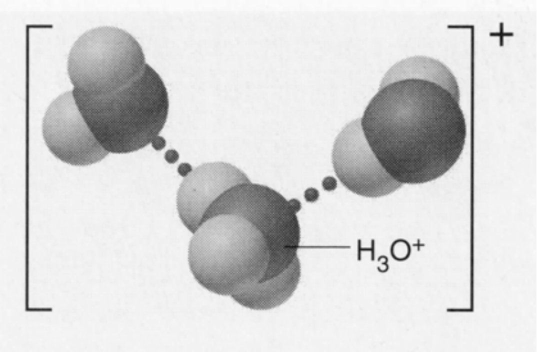
- Water self-ionizes:

$$K_w = \frac{\{H^+\}\{OH^-\}}{\cancel{\{H_2O\}} \rightarrow 1.0}$$

- $K_w = 10^{-14}$ at 25°C
- Neutral condition satisfied where $\{H^+\} = \{OH^-\} = 10^{-7}$ (pH = 7)
- pH 7 is dividing line between acidic & basic conditions
  - At pH < 7, $\{H^+\} > 10^{-7}$, so $\{OH^-\} < 10^{-7}$ to maintain K_w
- pH 7 is not always neutral:
- K_w changes with temp:
  - $K_w = 55 \times 10^{-14} = 10^{-12.26}$ at 100°C
  - Neutral pH where $\{H^+\} = \{OH^-\} = 10^{-6.13}$
  - pH 6.5 acidic at one temp, basic at another

pH 6.13 is neutral

$\{H^+\} = \{H_3O^+\}$



- Usually use $\{H^+\}$ to represent activity of free H^+ ions
- H^+ typically associated with one or more H_2O mCs
  - H_3O+ (hydronium ion)
  - True situation: $pH = -\log_{10}\{H_3O^+\}$

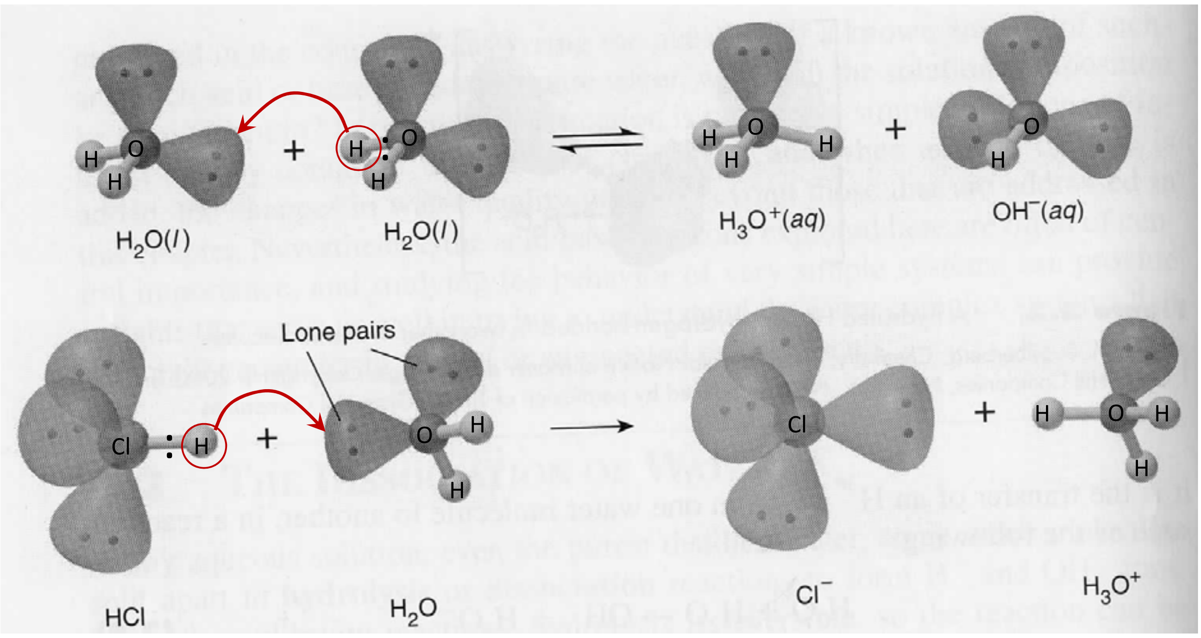
- Implication) Sometimes write acid-base rxns as dissociation of H^+:

$$H_2O \leftrightarrow H^+ + OH^- \quad \text{and} \quad HA \leftrightarrow H^+ + A^-$$

- Real reaction involves transfer of H^+ from acid to base mCs:

$$H_2O + H_2O \leftrightarrow H_3O^+ + OH^- \quad \text{and} \quad HA + H_2O \leftrightarrow H_3O^+ + A^-$$

Acid-Base Rxns = H^+ exchange rxns



From Benjamin (2002) Water Chemistry (Fig. 3.3)

Does it matter fo ?

Take Home Message: In this class,

1. $\{H_3O^+\}$ and $\{H^+\}$ mean same thing
2. Acid-base reactions may be presented either as dissociations or H^+ transfer rxns to/from H_2O

- Answer: **No**
- Algebraically, express
  - A. $\{H^+\}$ and $\{H_3O^+\}$ mean the same thing
  - B. $\{H_2O\} = 1.0$

$$K_w = \frac{\overset{\nearrow = \{H_3O^+\}}{\{H^+\}}\{OH^-\}}{\underset{\searrow 1.0}{\{H_2O\}}} = \frac{\overset{\nearrow = \{H^+\}}{\{H_3O^+\}}\{OH^-\}}{\underset{\searrow 1.0}{\{H_2O\}^2}} = 10^{-14}$$

$$K_a = \frac{\overset{\nearrow = \{H_3O^+\}}{\{H^+\}}\{A^-\}}{\{HA\}} = \frac{\overset{\nearrow = \{H^+\}}{\{H_3O^+\}}\{A^-\}}{\{HA\}\underset{\searrow 1.0}{\{H_2O\}}}$$

Definitions of Acids and Bases

- **Classic definition:** Bronsted acids and bases
  - Acid: molecules that can donate a H^+ (to water)
  - Base: molecules that can accept a H^+ (from water)

$$\underset{\text{Acid}}{HA} \leftrightarrow H^+ + \underset{\text{Base}}{A^-}$$

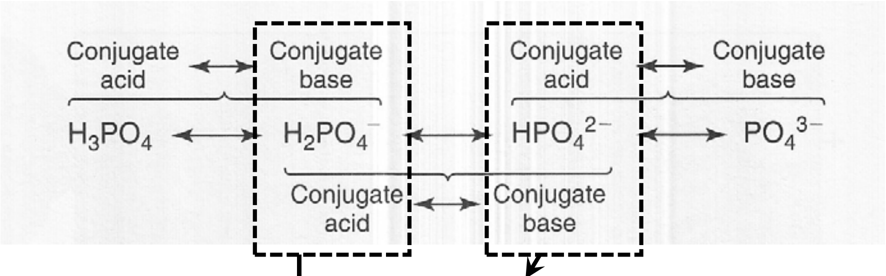
$$\underset{\text{Acid}}{HA} + \underset{\text{Base}}{H_2O} \leftrightarrow \underset{\text{Acid}}{H_3O^+} + \underset{\text{Base}}{A^-}$$

- When an acid molecule donates a H^+ to H_2O, it generates a corresponding base (can accept a H^+ from H_2O to reform the acid)

- HA / A^-: conjugate acid/base pair

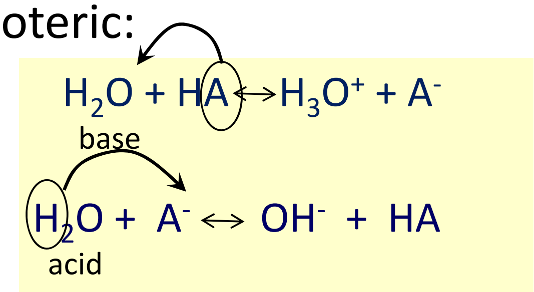
Conjugate acid/base pairs

- Phosphate:
  - Phosphoric acid (H_3PO_4): **triprotic acid** (3 acid-labile H^+)
  - 3 conjugate acid/base pairs



H_2PO_4 and HPO_4^{2-} **amphoteric** – can act as either a conj. acid or conj. base

- Water is amphoteric:



$$\underset{\text{base}}{H_2O} + HA \leftrightarrow H_3O^+ + A^-$$

$$\underset{\text{acid}}{H_2O} + A^- \leftrightarrow OH^- + HA$$

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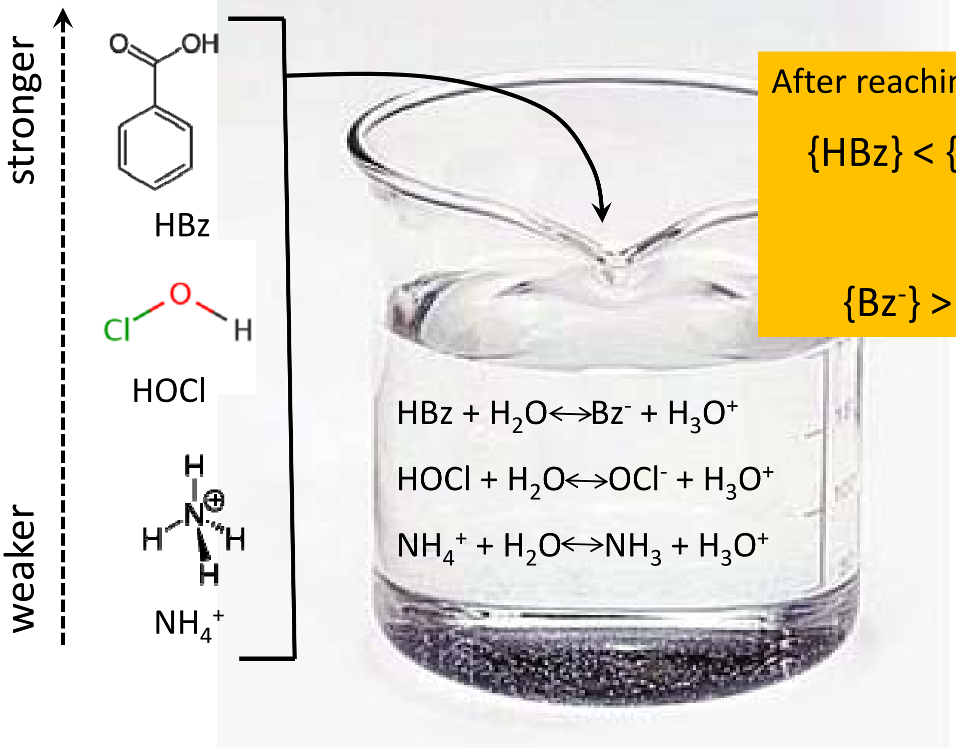
Acid strength: tendency to donate a H^+ to H_2O

- Consider adding equal conc. of 3 acids to a beaker of water



$HBz + H_2O \leftrightarrow Bz^- + H_3O^+$

$HOCl + H_2O \leftrightarrow OCl^- + H_3O^+$

$NH_4^+ + H_2O \leftrightarrow NH_3 + H_3O^+$

After reaching equilibrium:

$\{HBz\} < \{HOCl\} < \{NH_4^+\}$

and

$\{Bz^-\} > \{OCl^-\} > \{NH_3\}$

Acid strength (cont.)

- K_a: quantitative measure of acid strength

$$K_a = \frac{\{H^+\}\{A^-\}}{\{HA\}} = \frac{\{H^+\}\gamma_{-1}[A^-]}{\gamma_0[HA]}$$

- As K_a ↑, tendency to dissociate (or donate H^+ to H_2O) ↑
- Often, K_a values listed in terms of pK_a

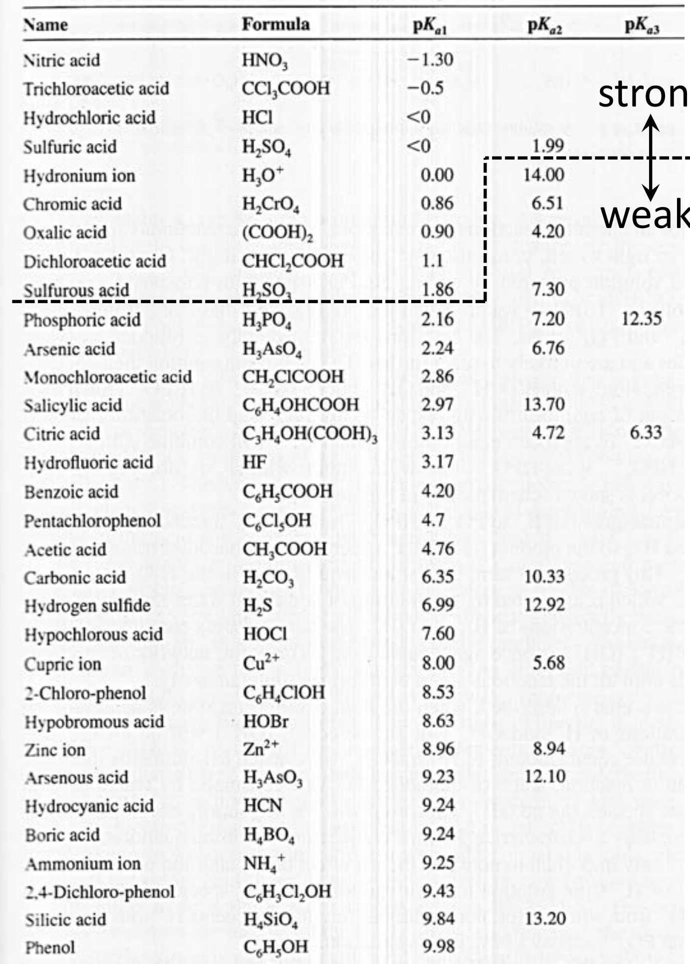
$$pK_a = -\log K_a$$

Acid	K_a	pK_a
HBz (benzoic acid)	$10^{-4.2}$	4.20
HOCl (hypochlorous acid)	$10^{-7.6}$	7.60
NH_4^+ (ammonium)	$10^{-9.25}$	9.25

↑ stronger

weaker

- Larger K_a correspond to lower pK_a
  - Like higher $\{H^+\}$ corresponds to lower pH



Name	Formula	pK_{a1}	pK_{a2}	pK_{a3}
Nitric acid	HNO_3	−1.30		
Trichloroacetic acid	CCl_3COOH	−0.5		
Hydrochloric acid	HCl	<0		
Sulfuric acid	H_2SO_4	<0	1.99	
Hydronium ion	H_3O^+	0.00	14.00	
Chromic acid	H_2CrO_4	0.86	6.51	
Oxalic acid	$(COOH)_2$	0.90	4.20	
Dichloroacetic acid	$CHCl_2COOH$	1.1		
Sulfurous acid	H_2SO_3	1.86	7.30	
Phosphoric acid	H_3PO_4	2.16	7.20	12.35
Arsenic acid	H_3AsO_4	2.24	6.76	
Monochloroacetic acid	$CH_2ClCOOH$	2.86		
Salicylic acid	$C_6H_4OHCOOH$	2.97	13.70	
Citric acid	$C_3H_4OH(COOH)_3$	3.13	4.72	6.33
Hydrofluoric acid	HF	3.17		
Benzoic acid	C_6H_5COOH	4.20		
Pentachlorophenol	C_6Cl_5OH	4.7		
Acetic acid	CH_3COOH	4.76		
Carbonic acid	H_2CO_3	6.35	10.33	
Hydrogen sulfide	H_2S	6.99	12.92	
Hypochlorous acid	HOCl	7.60		
Cupric ion	Cu^{2+}	8.00	5.68	
2-Chloro-phenol	C_6H_4ClOH	8.53		
Hypobromous acid	HOBr	8.63		
Zinc ion	Zn^{2+}	8.96	8.94	
Arsenous acid	H_3AsO_3	9.23	12.10	
Hydrocyanic acid	HCN	9.24		
Boric acid	H_4BO_4	9.24		
Ammonium ion	NH_4^+	9.25		
2,4-Dichloro-phenol	$C_6H_3Cl_2OH$	9.43		
Silicic acid	H_4SiO_4	9.84	13.20	
Phenol	C_6H_5OH	9.98		

strong

weak

pKa ≈ 2

- Mono- and multiprotic acids
- Varying strength: varying tendency to dissociate
- Not all protons can dissociate at relevant pH values
- Strong acid assumption: we assume complete dissociation when added to water
- Weak acids: only partial dissociation

Table 3.2 in Benjamin 2002. Water Chemistry

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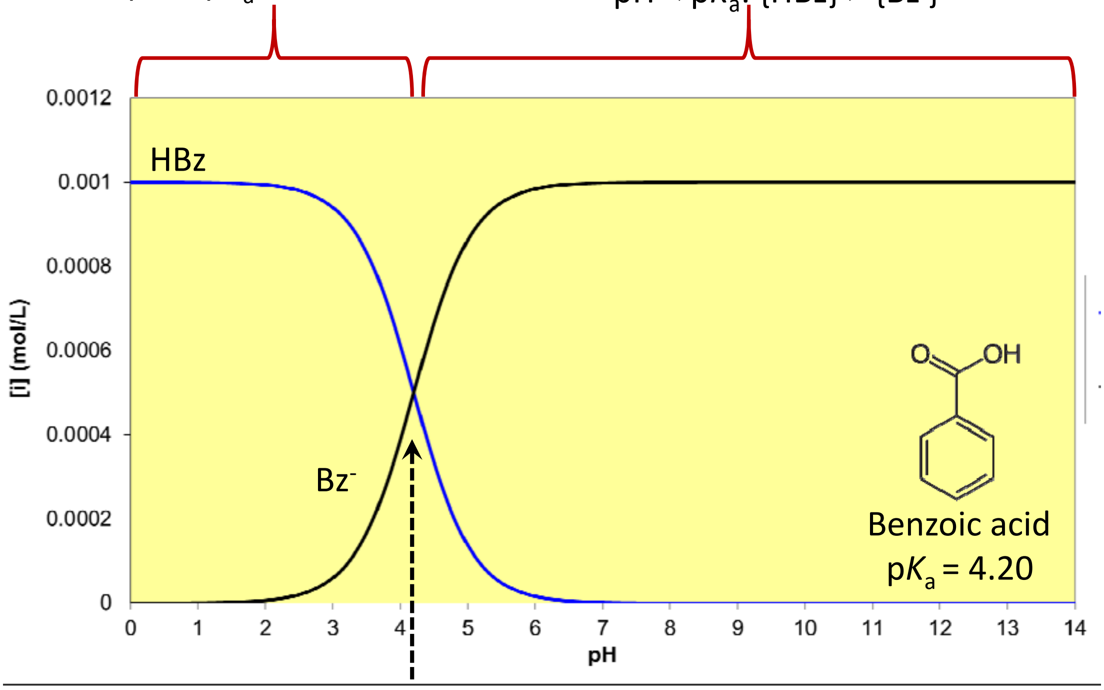
- $\mathrm{p}K_a$ = pH where {conj. acid} = {conj. base}

pH > $\mathrm{p}K_a$: {HBz} < {Bz$^-$}

pH < $\mathrm{p}K_a$: {HBz} > {Bz$^-$}



Benzoic acid
$\mathrm{p}K_a$ = 4.20

pH = $\mathrm{p}K_a$

Multiprotic acid equilibria

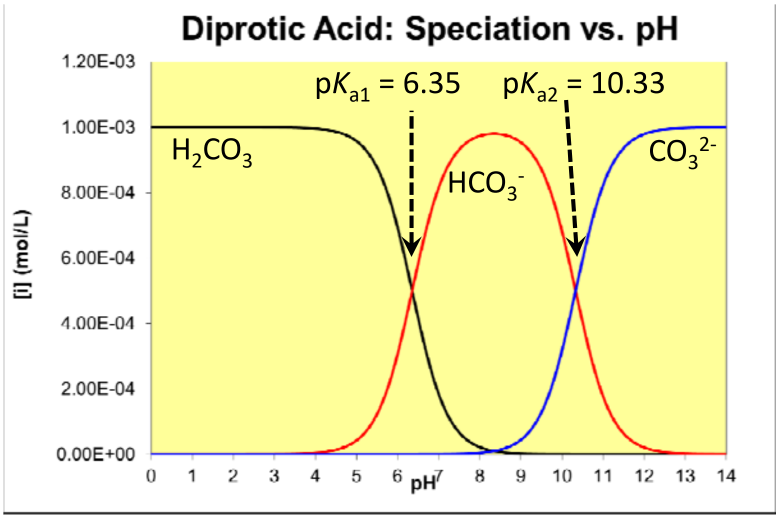
- Some acids can donate multiple H^+ to water
  - E.g., phosphoric(H_3PO_4), carbonic (H_2CO_3), arsenous (H_3AsO_3) acids
  - pK_{a1}, pK_{a2}, etc...used to characterize successive dissociations
- Carbonic acid:

$H_2CO_3 \leftrightarrow H^+ + HCO_3^-$

$$K_{a1} = 10^{-6.35} = \frac{\{H^+\}\{HCO_3^-\}}{\{H_2CO_3\}}$$

$HCO_3^- \leftrightarrow H^+ + CO_3^{2-}$

$$K_{a2} = 10^{-10.33} = \frac{\{H^+\}\{CO_3^{2-}\}}{\{HCO_3^-\}}$$



Expressing acid-base speciation as a function of pH

- **Goal:** We'd like to obtain an expression for the fractional concentrations of the conjugate acid and base in terms of the **solution pH** and the $\boldsymbol{K_a}$ of the acid-base conjugate pair

- Solution: solve for fractional concentration of individual species, α_i, by manipulating mass balance + K_a relationships, e.g., for acetic acid (pK_a = 4.76):

$$\alpha_0 = \frac{[\mathrm{HAc}]}{C_{T,A}}$$

$C_{T,Ac}$ = [HAc] + [Ac^-]

$$K_a = \frac{[Ac^-]\{H^+\}}{[HAc]}$$

- Rearrange the equilibrium expression to solve for the concentration of the conjugate base:

$$[Ac^-] = [HAc]\frac{K_a}{\{H^+\}}$$

Expressing acid-base speciation as a function of pH

- Now, we plug this expression back into the mass balance expression

$$C_{T,Ac} = [HAc] + [HAc]\frac{K_a}{\{H^+\}} = [HAc](1 + \frac{K_a}{\{H^+\}})$$

- We can then solve for α_0:

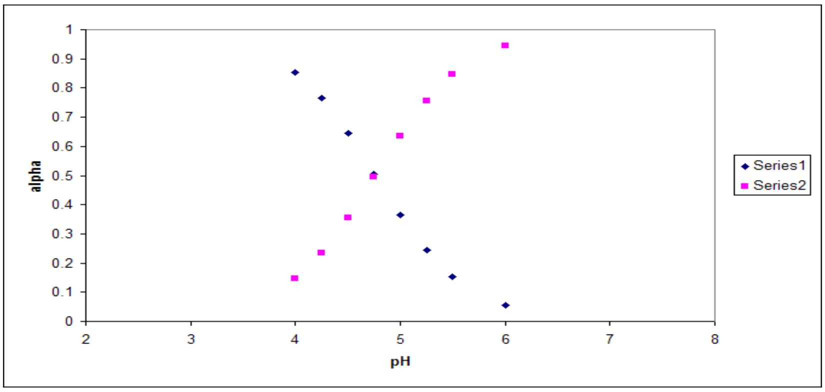
$$\alpha_0 = \frac{[HAc]}{C_{T,Ac}} = \frac{1}{1 + \frac{K_a}{\{H^+\}}}$$

- Using the same procedure, we can solve for α_1:

$$\alpha_1 = \frac{[Ac^-]}{C_{T,Ac}} = \frac{1}{\frac{\{H^+\}}{K_a} + 1}$$

- We can then plug these expressions into spreadsheet and calculate the acid-base speciation as a function of pH

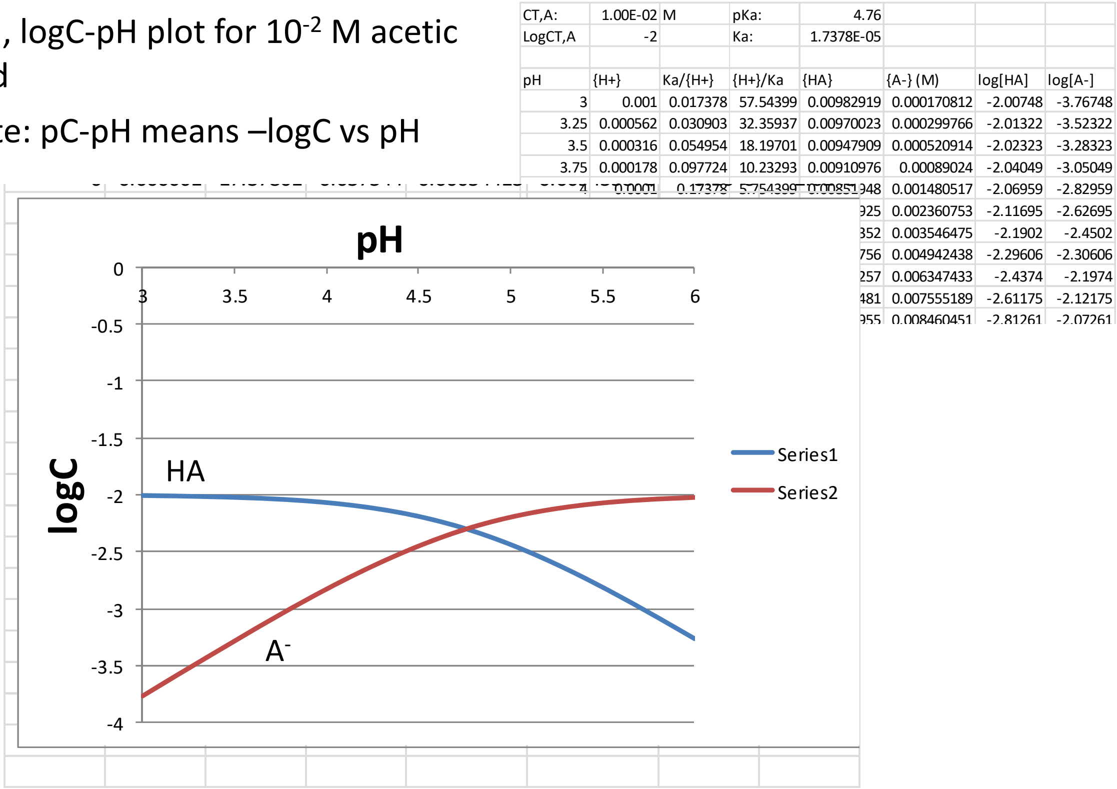
pH	{H+}	Ka/{H+}	{H+}/Ka	αo	α1
4	0.0001	0.1737801	5.754399	0.851948	0.148052
4.25	5.62E-05	0.3090295	3.235937	0.763925	0.236075
4.5	3.16E-05	0.5495409	1.819701	0.645352	0.354648
4.75	1.78E-05	0.9772372	1.023293	0.505756	0.494244
5	0.00001	1.7378008	0.57544	0.365257	0.634743
5.25	5.62E-06	3.0902954	0.323594	0.244481	0.755519
5.5	3.16E-06	5.4954087	0.18197	0.153955	0.846045
6	0.000001	17.378008	0.057544	0.054413	0.945587



- Normal-scale α vs pH plots emphasize speciation trends when pH near pK_a
- Visualizing the α vs pH plots is sometimes useful to help make simplifying assumptions when solving equilibrium problems

Many times it is more useful to examine speciation trends on a logarithmic scale

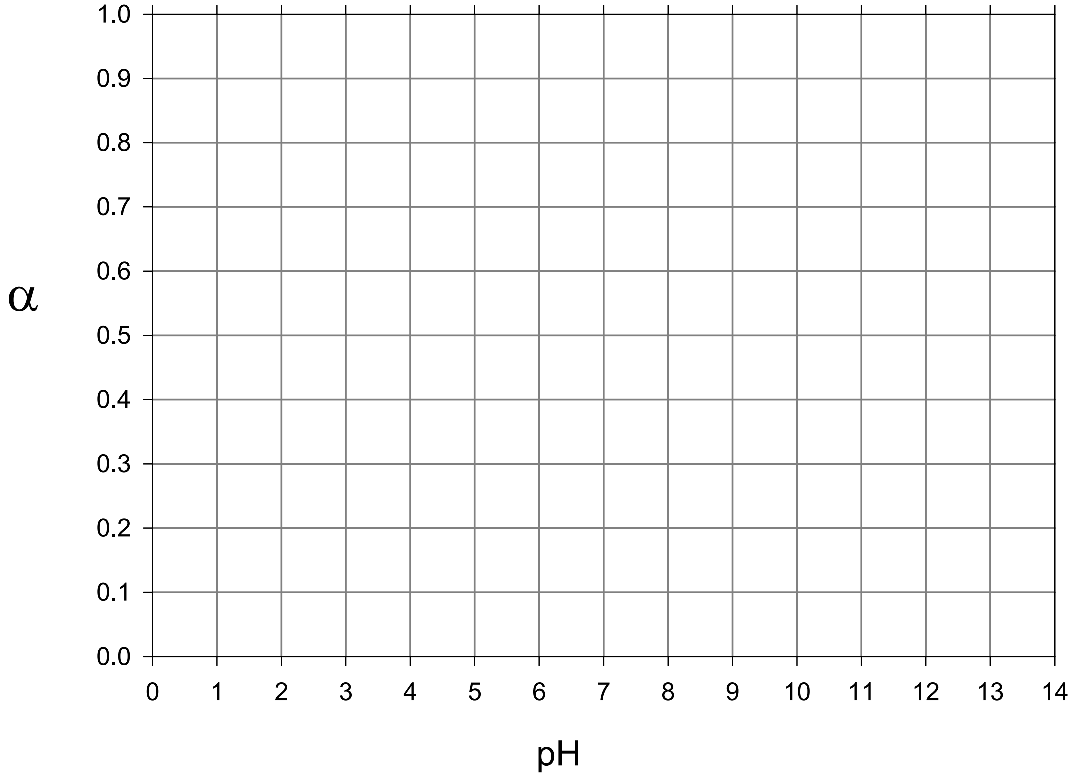
- E.g., logC-pH plot for 10^{-2} M acetic acid
- Note: pC-pH means –logC vs pH



CT,A:	1.00E-02	M	pKa:	4.76			
LogCT,A	-2		Ka:	1.7378E-05			
pH	{H+}	Ka/{H+}	{H+}/Ka	{HA}	{A-} (M)	log[HA]	log[A-]
3	0.001	0.017378	57.54399	0.00982919	0.000170812	-2.00748	-3.76748
3.25	0.000562	0.030903	32.35937	0.00970023	0.000299766	-2.01322	-3.52322
3.5	0.000316	0.054954	18.19701	0.00947909	0.000520914	-2.02323	-3.28323
3.75	0.000178	0.097724	10.23293	0.00910976	0.00089024	-2.04049	-3.05049
4	0.0001	0.17378	5.754399	0.00851948	0.001480517	-2.06959	-2.82959
				925	0.002360753	-2.11695	-2.62695
				352	0.003546475	-2.1902	-2.4502
				756	0.004942438	-2.29606	-2.30606
				257	0.006347433	-2.4374	-2.1974
				481	0.007555189	-2.61175	-2.12175
				955	0.008460451	-2.81261	-2.07261

- Can calculate using a generic spreadsheet with a p*K*a and $C_{T,A}$ value
- Can quickly sketch on paper or in your head using a few rule:
  - (1) At pH = pKa, [HA] = [A^-] = $0.5C_{t,a}$ if we are talking about an equilibrium only between a single acid-base conjugate pair
  - (2) At pH = (pK_a–1): [HA]/[A-] = 10 and At pH = (pK_a+1): [HA]/[A-] = 0.1
  - (3) For normal-scale plots, back of the envelope-wise, we can do like we did for benzoic acid, and draw the expected curves for an exponential changes in concentration as we approach the pKa from both sides.

E.g., for 10^{-3} M hypochlorous acid ($pK_a = 7.5$)



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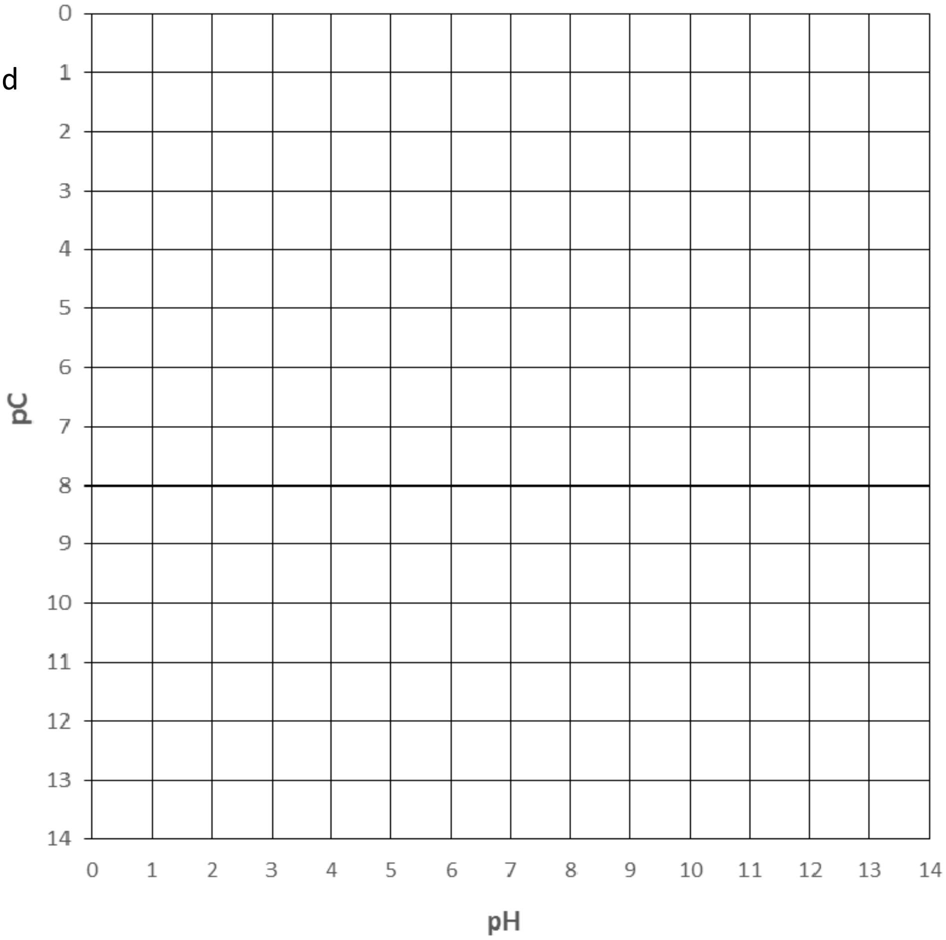
4. For pC-pH plots, First add a horizontal line for $pC_{T,A}$
5. Add a point at pH = pK_a for $[HA] = [A^-] = 0.5C_{T,A}$ = ~0.3 log units below $pC_{T,A}$ line
6. Rule: slopes the lines for the conjugate base will always differ from the conjugate acid by +1
7. When pH is more than 1 unit below the pKa, $pC_{HA} = pC_{T,A}$ (and slope of $pC_{HA} = 0$; so slope of $pC_{A-} = +1$)
8. When pH is more than 1 unit above the pKa, $pC_{A-} \approx pC_{T,A}$ (and slope of $pC_{A-} = 0$; so slope of $pC_{HA} = -1$)

E.g., for 10^{-3} M hypochlorous acid ($pK_a = 7.5$)



We can extend the same set of rules for more complex multiprotic acids like carbonic acid (H_2CO_3*)

$$C_{T,CO3} = [H_2CO_3^*] + [HCO_3^-] + [CO_3^{2-}]$$

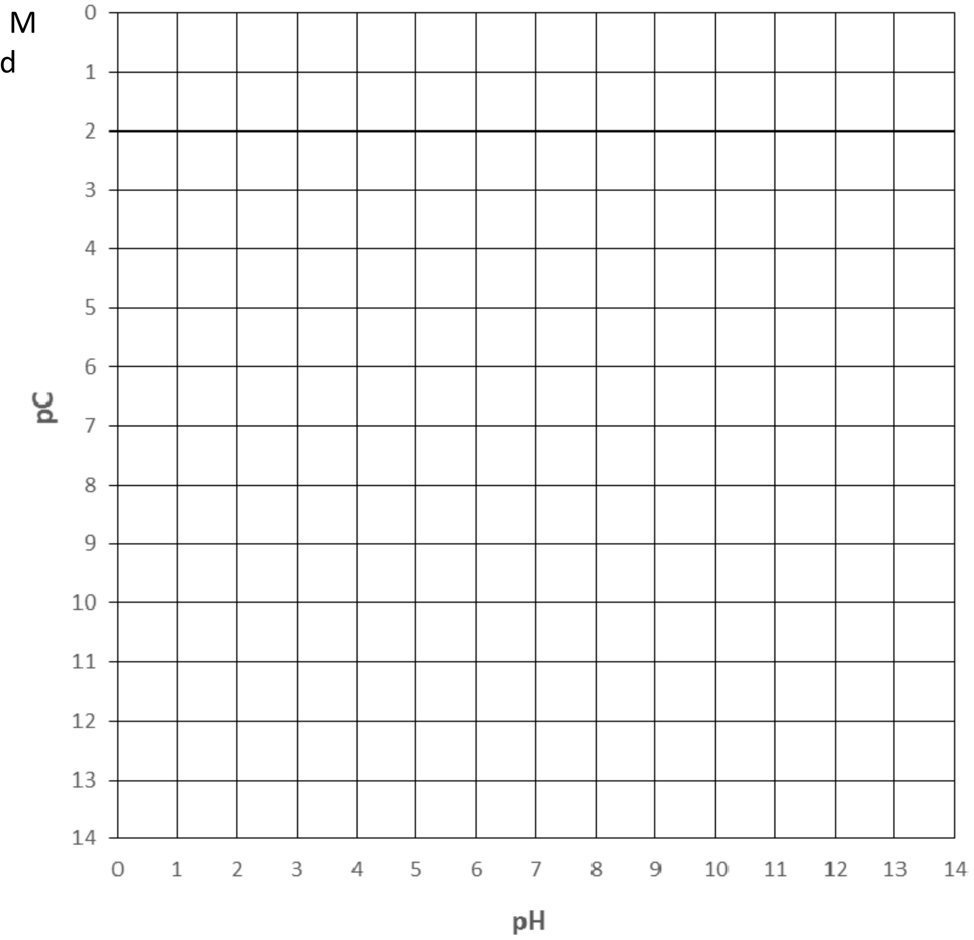
$$H_2CO_3^* + H_2O = HCO_3^- + H_3O^+ \qquad pK_{a1} = 6.35$$

$$HCO_3^- + H_2O = CO_3^{2-} + H_3O^+ \qquad pK_{a2} = 10.33$$

Extensions:

4. If pKa values are >2 units apart, treat as 2 conjugate acid base pairs.
5. Always keep in mind that the slope of the conjugate base is always +1 relative to its conjugate acid

E.g., for 10^{-5} M carbonic acid



We can also make extensions of our calculations to obtain expressions for α values

$$\alpha_0 = \frac{[H_2CO_3*]}{C_{T,CO3}} =$$

- Divide through by $[H_2CO_3^*]$:

$$\alpha_0 = \frac{[H_2CO_3^*]/[H_2CO_3^*]}{[H_2CO_3^*]/[H_2CO_3^*]+[HCO_3^-]/[H_2CO_3^*]+[CO_3^{2-}]/[H_2CO_3^*]}$$

$$\alpha_0 = \frac{1}{1+[HCO_3^-]/[H_2CO_3^*]+[CO_3^{2-}]/[H_2CO_3^*]}$$

- From the equilibrium acid dissociation expressions:

$$K_{a1} = \frac{\{H^+\}[HCO_3^-]}{[H_2CO_3*]} \therefore$$

and:

$$K_{a1}K_{a2} = \frac{\{H^{+}\}[HCO_3^{-}]}{[H_2CO_3*]}\frac{\{H^{+}\}[CO_3^{2-}]}{[HCO_3^{-}]} \therefore$$

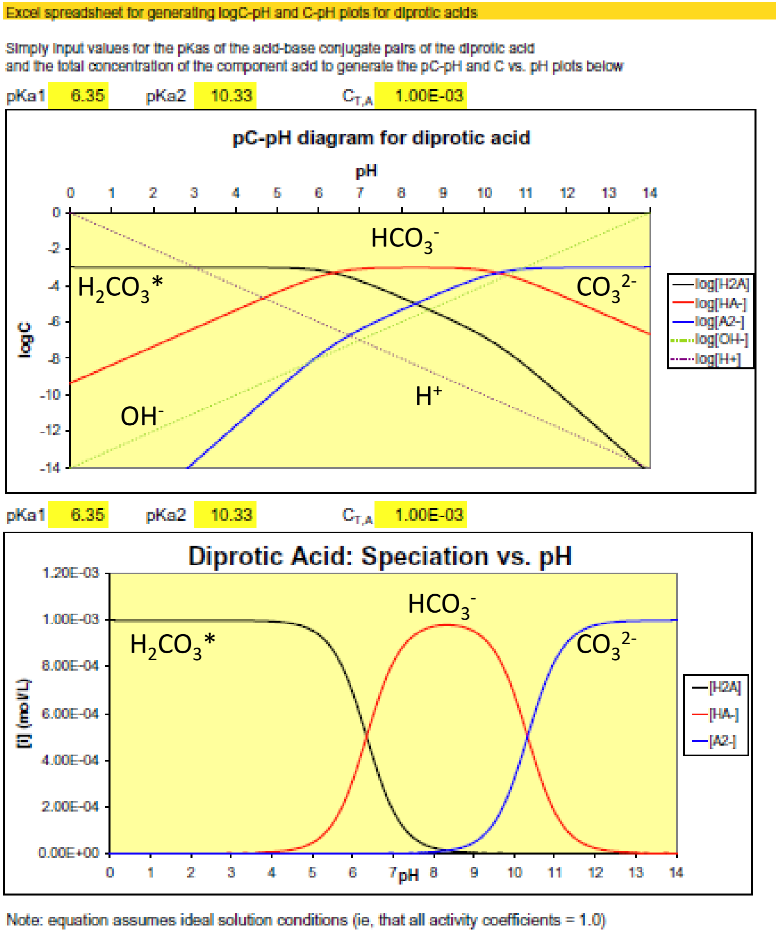
So:

$$\alpha_0 = \frac{1}{1 + \frac{K_{a1}}{\{H^+\}} + \frac{K_{a1}K_{a2}}{\{H^+\}^2}}$$

Similarly:

$$\alpha_1 = \frac{1}{\frac{\{H^+\}}{K_{a1}} + 1 + \frac{K_{a2}}{\{H^+\}}}$$

$$\alpha_2 = \frac{1}{\frac{\{H^+\}^2}{K_{a1}K_{a2}} + \frac{\{H^+\}}{K_{a2}} + 1}$$



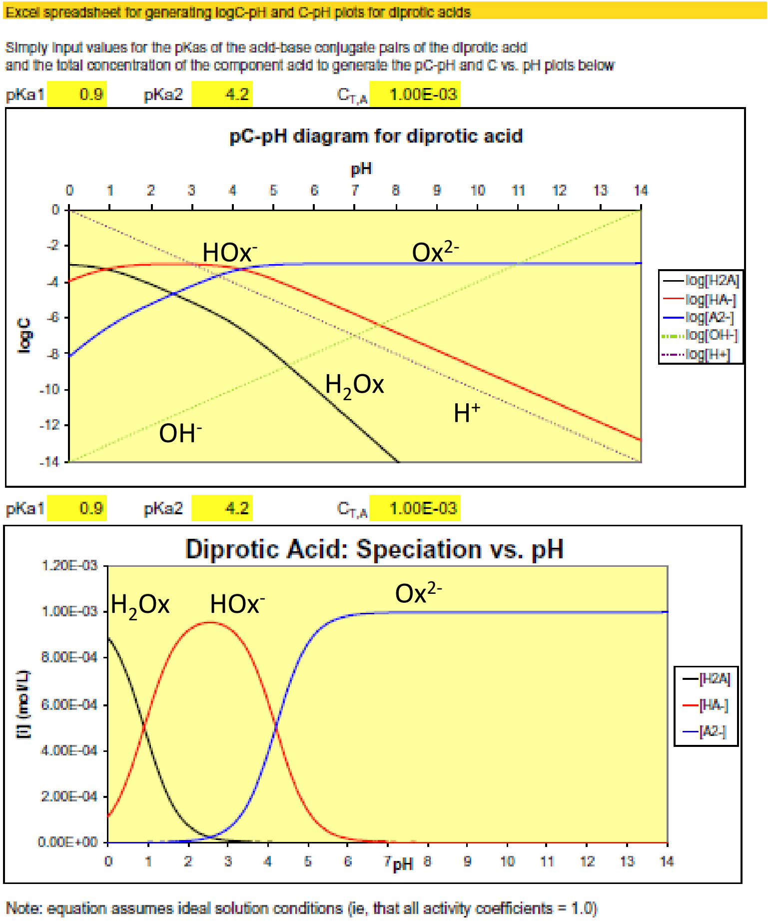
Excel spreadsheet for generating logC-pH and C-pH plots for diprotic acids

Simply input values for the pKas of the acid-base conjugate pairs of the diprotic acid
and the total concentration of the component acid to generate the pC-pH and C vs. pH plots below

pKa1 6.35 pKa2 10.33 $C_{T,A}$ 1.00E-03

pKa1 6.35 pKa2 10.33 $C_{T,A}$ 1.00E-03

Note: equation assumes ideal solution conditions (ie, that all activity coefficients = 1.0)



Excel spreadsheet for generating logC-pH and C-pH plots for diprotic acids

Simply input values for the pKas of the acid-base conjugate pairs of the diprotic acid
and the total concentration of the component acid to generate the pC-pH and C vs. pH plots below

pKa1	0.9	pKa2	4.2	$C_{T,A}$	1.00E-03

pKa1	0.9	pKa2	4.2	$C_{T,A}$	1.00E-03

Note: equation assumes ideal solution conditions (ie, that all activity coefficients = 1.0)

Expressing acid-base speciation as a function of pH

$$K_a = \frac{[Ac^-]\{H^+\}}{[HAc]}$$

$C_{T,Ac}$ = [HAc] + [Ac$^-$]

$$\alpha_0 = \frac{[HAc]}{C_{T,Ac}} = \frac{1}{1+\frac{K_a}{\{H^+\}}}$$

$$\alpha_1 = \frac{[Ac^-]}{C_{T,Ac}} = \frac{1}{\frac{\{H^+\}}{K_a}+1}$$

We can also make extensions of our calculations to obtain expressions for α values

$$\alpha_0 = \frac{[H_2CO_3*]}{C_{T,CO3}} =$$

- Divide through by [$H_2CO_3^*$] :

$$\alpha_0 = \frac{[H_2CO_3^*]/[H_2CO_3^*]}{[H_2CO_3^*]/[H_2CO_3^*]+[HCO_3^-]/[H_2CO_3^*]+[CO_3^{2-}]/[H_2CO_3^*]}$$

$$\alpha_0 = \frac{1}{1+[HCO_3^-]/[H_2CO_3^*]+[CO_3^{2-}]/[H_2CO_3^*]}$$

- From the equilibrium acid dissociation expressions:

$$K_{a1} = \frac{\{H^+\}[HCO_3^-]}{[H_2CO_3*]} \therefore$$

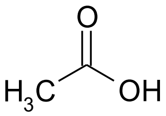
Today

- Review of Acid-Base Chem
- Acid-base speciation vs. pH
- **Introduction to solving simple acid speciation equilibrium problems**

Problem 1. Calculate the equilibrium pH and speciation of acetate after 10^{-3} M acetic acid is added to deionized water (nothing else initially present in the water). *Assume dilute solution approximates "infinite dilution" reference state condition.*

Step 1: List all the components in the system

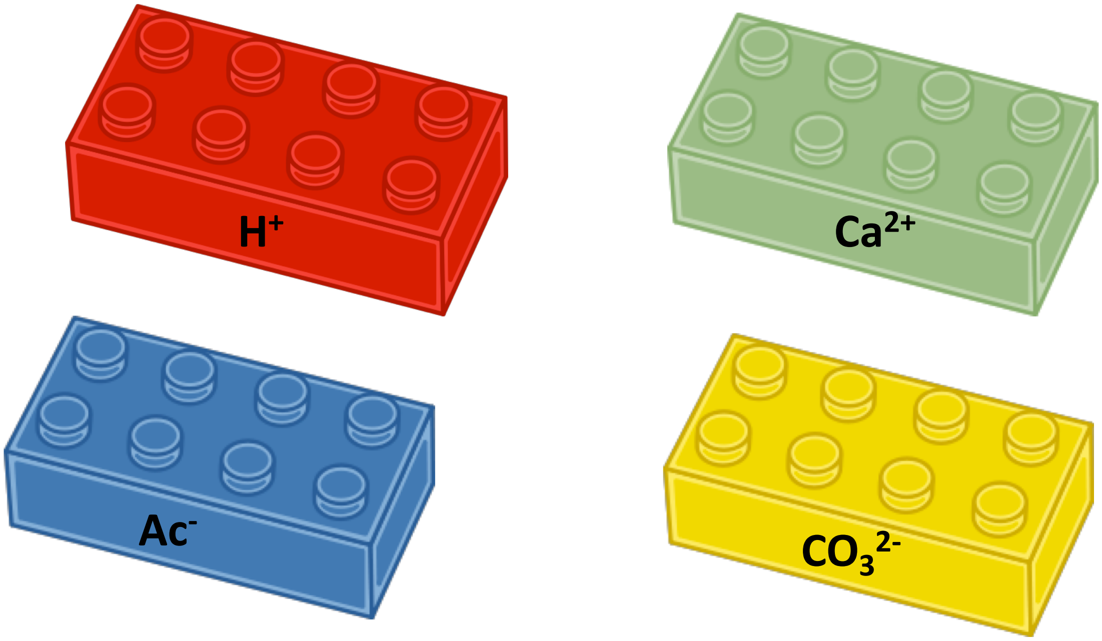
Acetic Acid



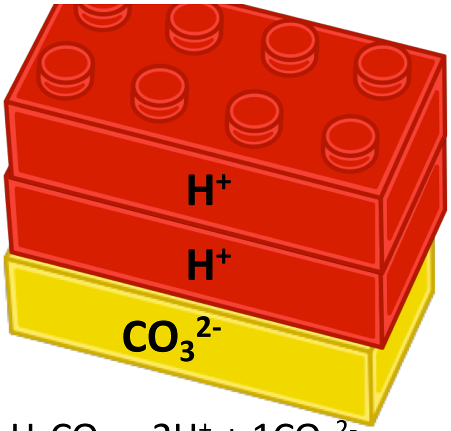
pK_a = 4.7

Step 2: List all the species that can be formed by combinations of components (include the "component" species as well)

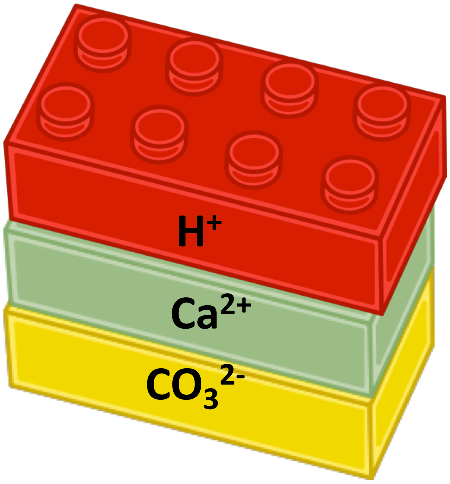
Components vs. Species



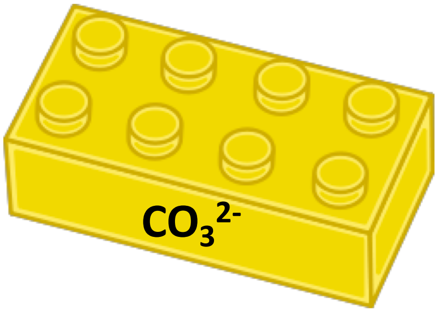
Components = irreducible parts
= pieces you combine to get species



$H_2CO_3 = 2H^+ + 1CO_3^{2-}$



$CaHCO_3^+ = 1Ca^{2+} + 1H^+ + 1CO_3^{2-}$



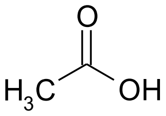
CO_3^{2-} = “component species”

Species = specific form of component
= formed by combination of component pieces

Problem 1. Calculate the equilibrium pH and speciation of acetate after 10^{-3} M acetic acid is added to deionized water (nothing else initially present in the water). *Assume dilute solution approximates "infinite dilution" reference state condition***.**

Step 1: List all the components in the system

Acetic Acid



$pK_a = 4.7$

Step 2: List all the species that can be formed by combinations of components (include the "component" species as well)

Step 3: List all the independent governing equations/mathematical constraints

Step 4: List all the other quantities that are known (e.g., total component conc., pH, concentration of any individual species)

Step 5: List all the quantities that remain unknown:

Step 6: Check – do we have as many independent governing equations as we have unknowns?

The Dreaded Step 7: Can we make any simplifying assumptions/guesses?

E.g., $[OH^-] << [H^+]$ (you guess that that equilibrium $pH \leq 6$) or $[H^+] << [OH^-]$ (you guess that eqbm $pH \geq 8$)

------Neglect $[OH^-]$ or $[H^+]$ in charge balance expression

Do you suspect that the concentration of any particular species is negligible in comparison to the concentration of one or more other species from the same component group?

---Neglect that species in the mass balance expression for the component or set the concentration of the "predominant" species of that component equal to C_T

---Neglect the concentration of that species in the charge balance expression only if the species from the same component with much higher concentration is also in the expression

Step 8: Solve the problem (using your simplifying assumptions):

Rearrange charge balance or mass balance expression to obtain a single equation with a single unknown (often choose $[H^+]$ or another master variable that appears in most expressions)

(a) Solve algebraically for unknown variable

(b) Solve by iteration (target term has to be one of the dominant terms in the expression)

Step 9A (do not omit): Check your assumptions!

Step 9b: If assumption is invalid, make a new (maybe opposite) assumption and repeat steps 8-9.

Problem 2: Calculate the equilibrium pH and speciation of chloride after 10^{-3} hydrochloric acid (HCl; pK_a = -3) is added to deionized water (nothing else initially present in the water). ***Assume dilute solution approximates "infinite dilution" assumption of the reference state.***

Step 1: components

Step 2: species

Step 3: equations

Step 4: knowns

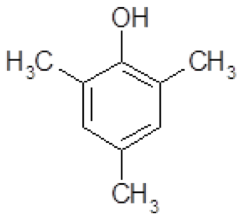
Step 5: unknowns

Step 6: #eqns ≥ unknowns?

Step 7: simplifying assumptions:

Step 8: Solve!

Step 9a: Check assumptions



Problem 3: Calculate the equilibrium pH and speciation of trimethylphenol (pK_a = 10.9) after 10^{-3} M is added to deionized water (nothing else initially present in the water). ***Assume dilute solution approximates "infinite dilution" assumption of the reference state.***

Step 1: components

Step 2: species

Step 3: equations

Step 4: knowns

Step 5: unknowns

Step 6: #eqns $\geq$ unknowns?

Step 7: simplifying assumptions:

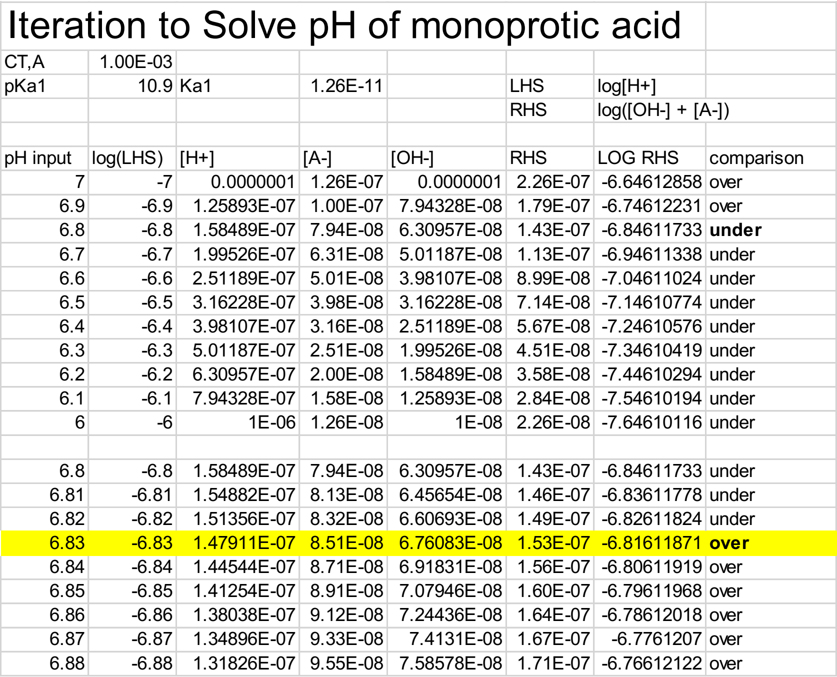
Step 8: Solve!

Step 9a: Check assumptions

Alternative: Solve for pH by iteration

Calculate charge balance at all pH values, compare Log(LHS) vs Log(RHS)

$$\log([H^+]) = \log([OH^-] + [\mathrm{Ph}^-])$$

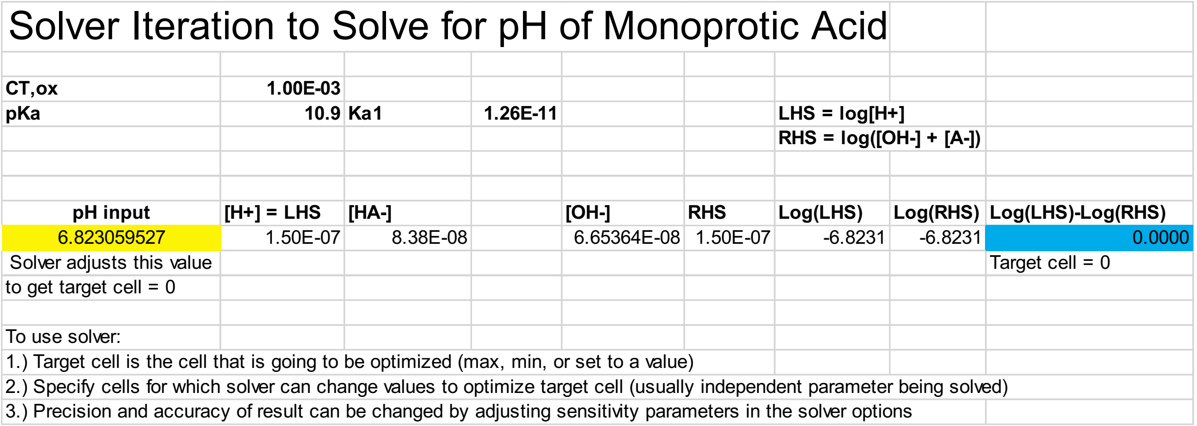


Iteration to Solve pH of monoprotic acid

CT,A	1.00E-03						
pKa1	10.9	Ka1	1.26E-11		LHS	log[H+]	
					RHS	log([OH-] + [A-])	
pH input	log(LHS)	[H+]	[A-]	[OH-]	RHS	LOG RHS	comparison
7	-7	0.0000001	1.26E-07	0.0000001	2.26E-07	-6.64612858	over
6.9	-6.9	1.25893E-07	1.00E-07	7.94328E-08	1.79E-07	-6.74612231	over
6.8	-6.8	1.58489E-07	7.94E-08	6.30957E-08	1.43E-07	-6.84611733	**under**
6.7	-6.7	1.99526E-07	6.31E-08	5.01187E-08	1.13E-07	-6.94611338	under
6.6	-6.6	2.51189E-07	5.01E-08	3.98107E-08	8.99E-08	-7.04611024	under
6.5	-6.5	3.16228E-07	3.98E-08	3.16228E-08	7.14E-08	-7.14610774	under
6.4	-6.4	3.98107E-07	3.16E-08	2.51189E-08	5.67E-08	-7.24610576	under
6.3	-6.3	5.01187E-07	2.51E-08	1.99526E-08	4.51E-08	-7.34610419	under
6.2	-6.2	6.30957E-07	2.00E-08	1.58489E-08	3.58E-08	-7.44610294	under
6.1	-6.1	7.94328E-07	1.58E-08	1.25893E-08	2.84E-08	-7.54610194	under
6	-6	1E-06	1.26E-08	1E-08	2.26E-08	-7.64610116	under
6.8	-6.8	1.58489E-07	7.94E-08	6.30957E-08	1.43E-07	-6.84611733	under
6.81	-6.81	1.54882E-07	8.13E-08	6.45654E-08	1.46E-07	-6.83611778	under
6.82	-6.82	1.51356E-07	8.32E-08	6.60693E-08	1.49E-07	-6.82611824	under
6.83	-6.83	1.47911E-07	8.51E-08	6.76083E-08	1.53E-07	-6.81611871	**over**
6.84	-6.84	1.44544E-07	8.71E-08	6.91831E-08	1.56E-07	-6.80611919	over
6.85	-6.85	1.41254E-07	8.91E-08	7.07946E-08	1.60E-07	-6.79611968	over
6.86	-6.86	1.38038E-07	9.12E-08	7.24436E-08	1.64E-07	-6.78612018	over
6.87	-6.87	1.34896E-07	9.33E-08	7.4131E-08	1.67E-07	-6.7761207	over
6.88	-6.88	1.31826E-07	9.55E-08	7.58578E-08	1.71E-07	-6.76612122	over

Or using the solver tool in Excel

$$\log([H^+]) = \log([OH^-] + [\text{Ph}^-])$$



Solver Iteration to Solve for pH of Monoprotic Acid								
CT,ox	**1.00E-03**							
pKa	**10.9**	**Ka1**	**1.26E-11**			**LHS = log[H+]**		
						RHS = log([OH-] + [A-])		
pH input	**[H+] = LHS**	**[HA-]**		**[OH-]**	**RHS**	**Log(LHS)**	**Log(RHS)**	**Log(LHS)-Log(RHS)**
6.823059527	1.50E-07	8.38E-08		6.65364E-08	1.50E-07	-6.8231	-6.8231	0.0000
Solver adjusts this value								Target cell = 0
to get target cell = 0								
To use solver:								
1.) Target cell is the cell that is going to be optimized (max, min, or set to a value)								
2.) Specify cells for which solver can change values to optimize target cell (usually independent parameter being solved)								
3.) Precision and accuracy of result can be changed by adjusting sensitivity parameters in the solver options								

Wrap up / Muddy Issues?