CH203 Lecture 3
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John. A. Porco, Jr.

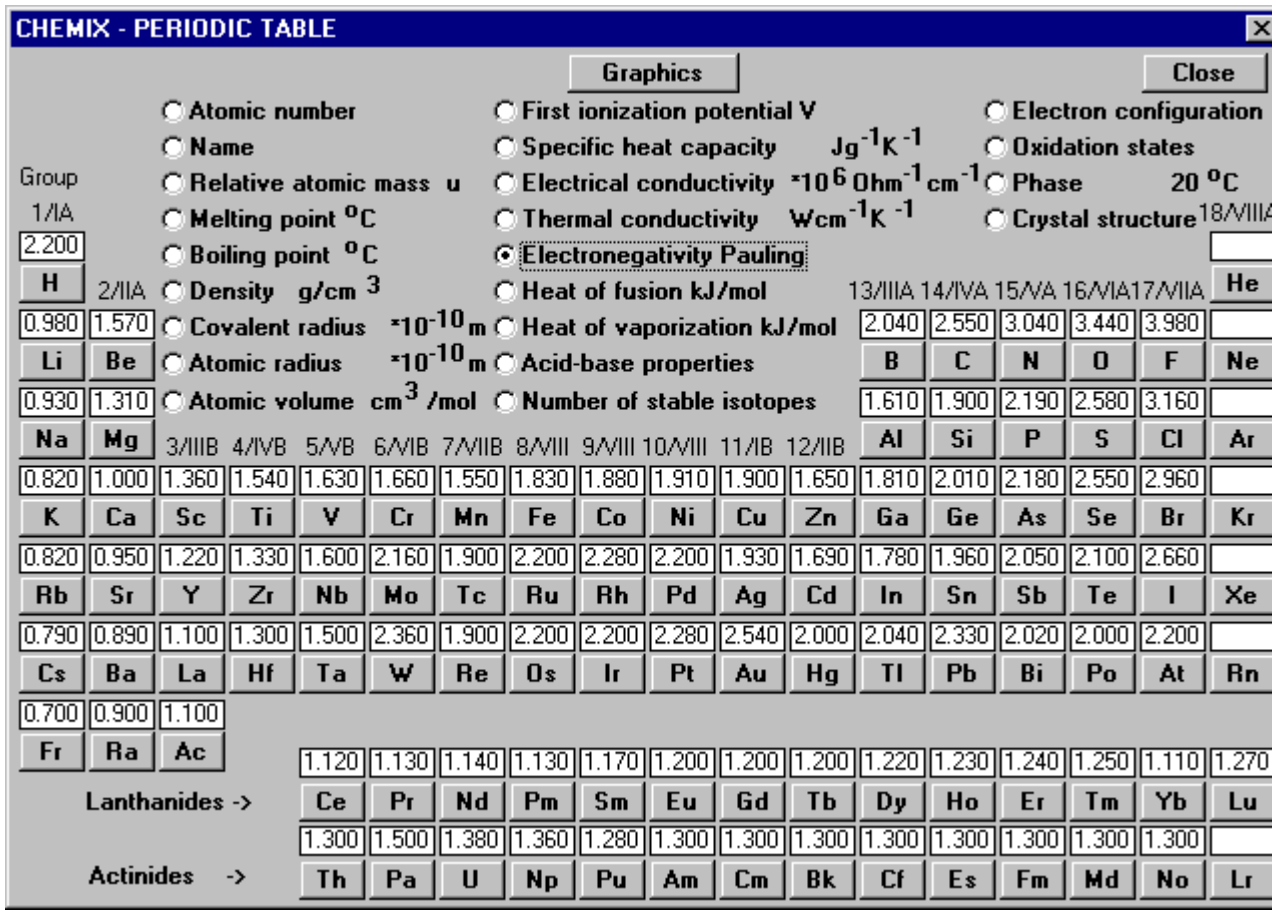
Department of Chemistry

porco@bu.edu

BOSTON UNIVERSITY

Review: Electronegativity

- Electronegativity is a measure of the tendency of an atom to attract a bonding pair of electrons.
- The Pauling scale is the most commonly used. Fluorine (the most electronegative element) is assigned a value of 4.0



http://www.standnes.no/chemix/periodictable/electronegativity-chart.gif

Bond Polarities

Bond	Diff in EN	Negative atom	Type of Bond
H - H	0.0	N/A	pure covalent
C - H	0.4	C	(weakly) polar covalent
O - H	1.4	O	polar covalent
H - F	1.9	F	polar covalent
S - O	1.0	O	polar covalent
C - O	1.0	O	polar covalent
Al - C	1.0	C	polar covalent
Na - Cl	2.1	Cl	ionic
Li - F	3.0	F	ionic
Mg - O	2.3	O	ionic
Mg - C	1.3	C	polar covalent

Similar EN's : *Nonpolar covalent*
Less than 2 EN units – *Polar covalent*
Greater than 2 EN units - *Ionic*

Example Format CH203 Notecards

Front

Title/Topic

Location Of Info.

Equations

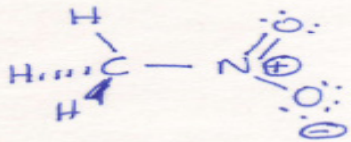
Formal Charge

Ch 2
Pg 34

Formal Charge = (# valence e⁻ free atom)
− (# valence e⁻ bound atom)

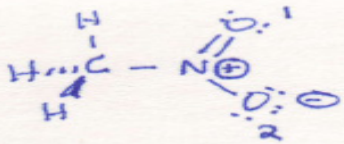
or

= (# valence e⁻) − (½ # bonding e⁻)
− (# nonbonding e⁻)



Nitromethane

Back



Practice

Formal charges:

C	← # valence e⁻ free atom →	N	O¹	O²
4		5	6	6
−4	← ½ bonding e⁻ →	−4	−2	−1
= 0	← Non-bonding e⁻ →	−0	−4	−6
= 0		+1	0	−1

Example Format CH203 Notecards

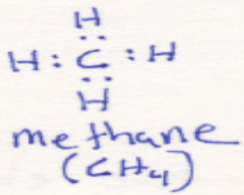
Front

Location Of Info.

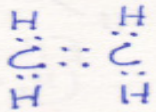
Title/Topic

Structural Representations

Ch 1 Pg 9



methane (CH_4)

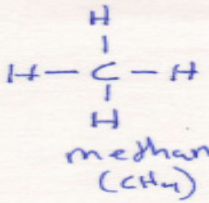


Ethylene (C_2H_4)

Definition

Lewis Dot Structure – Valence electrons of atoms are represented as dots. Shared e^-s appear between atoms; one pair of e^-s is one bond.

Back



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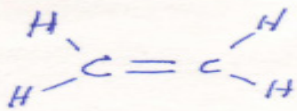


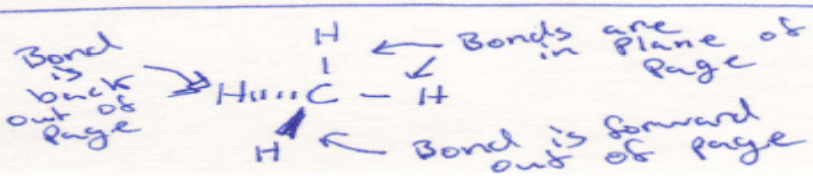
Ethylene (CH_2CH_2)

Practice

Kekulé or line bond structure – two-electron covalent bonds are indicated as a line drawn between atoms.

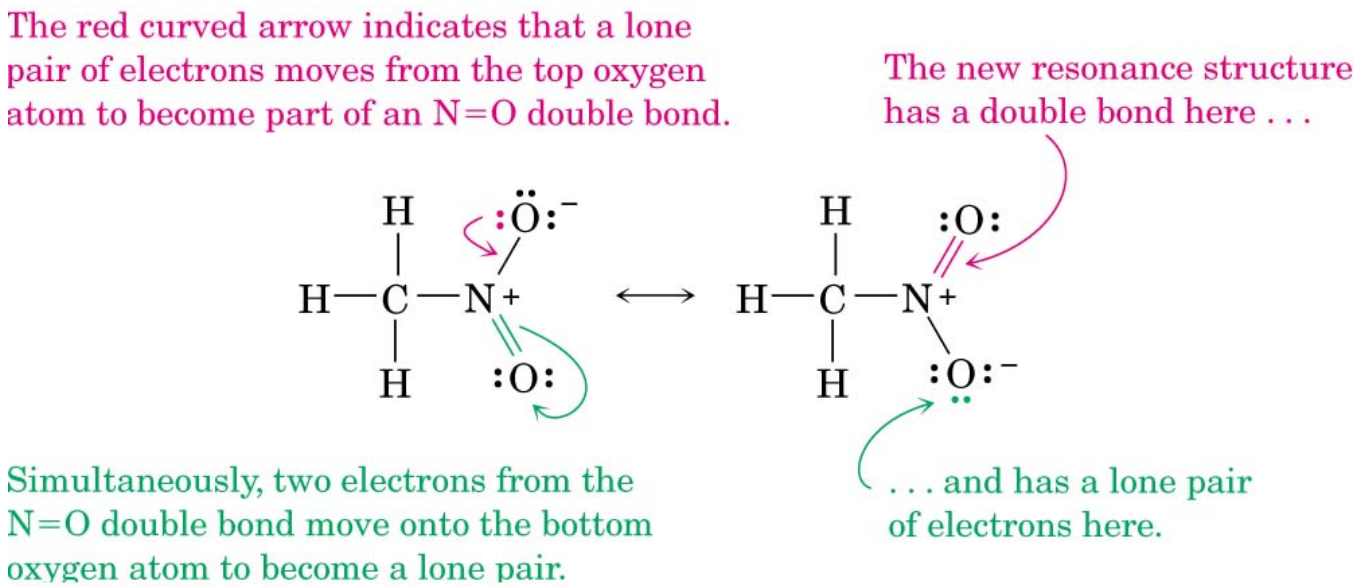
Also:

Additional Information



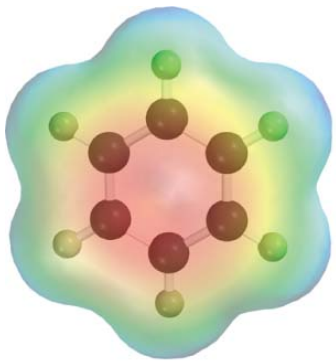
Curved Arrows and Resonance Forms

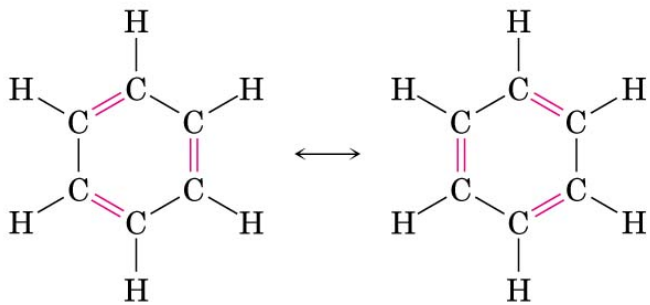
- We can imagine that electrons move in pairs to convert from one resonance form to another
- A curved arrow shows that a pair of electrons moves *from* the atom or bond at the tail of the arrow *to* the atom or bond at the head of the arrow



Resonance Hybrids

- A structure with resonance forms does not alternate between the forms
- Instead, it is a *hybrid* of the two resonance forms, so the structure is called a **resonance hybrid**
- For example, benzene (C_6H_6) has two resonance forms with alternating double and single bonds
  - In the resonance hybrid, the actual structure, all its C-C bonds equivalent, midway between double and single





Benzene (two resonance forms)

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Electronegativity

Bond Polarity

- Can use diff in Eneg btween 2 atoms to gauge polarity of bonding btwn them.

F_2

F – F

4.0 – 4.0 = 0

nonpolar covalent

H – F

H – F

4.0 – 2.1 = 1.9

polar covalent

$\delta+$ $\delta-$

H – F

or $H \xrightarrow{+} F$

Indicates direction of bond polarity

Li F

Li F

4.0 – 1.0 = 3.0

Ionic (non-covalent)

Formal Charge

closely rel. to bond polarity & dipole moment

Assign

Unit positive or negative charge of an atom

e⁻ "accounting"

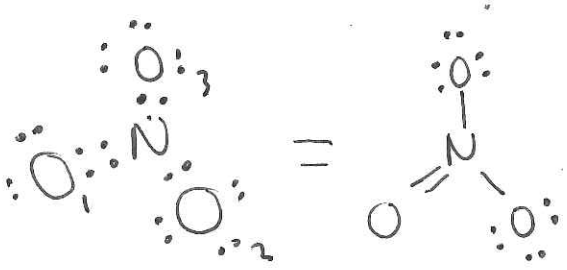
F.C = # val. e⁻s as a neutral free atom − # vale e⁻s in bound atom/state | # of atoms owned by that atom in a molecule

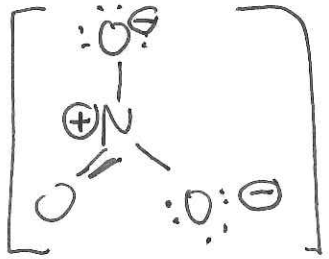
↓

same as group # on per. table

$$= (\#\ \text{val e}^-\text{s}) - \left(\begin{matrix}\text{half of}\\ \text{bond e}^-\text{s}\end{matrix}\right) - \left(\begin{matrix}\text{number of}\\ \text{nonbonding e}^-\text{s}\end{matrix}\right)$$

e.g. nitrate ion NO_3^-



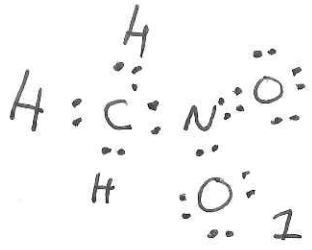


For N: $5 - \left(\frac{8}{4}\right) - 0 = +1$

For O_1: $6 - \left(\frac{4}{2}\right) - 4 = 0$

For O_2/O_3: $6 - \left(\frac{2}{2}\right) - 6 = -1$

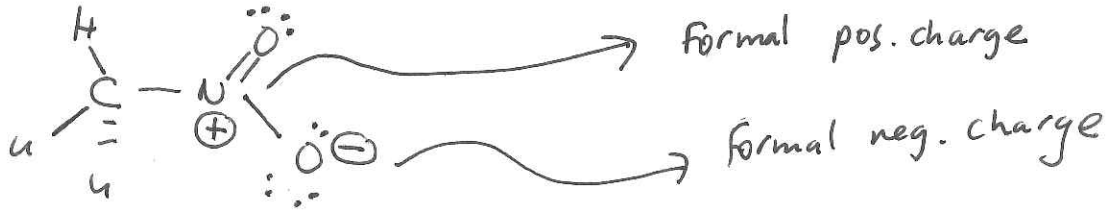
CH_3NO_2 =



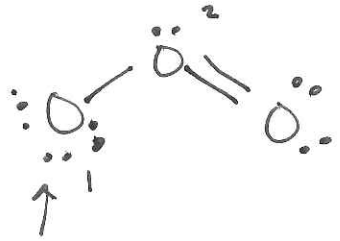
3

For N: $5 - \left(\frac{8}{2}\right) - 0 = +1$

O_1 $6 - \left(\frac{2}{2}\right) - 6 = -1$



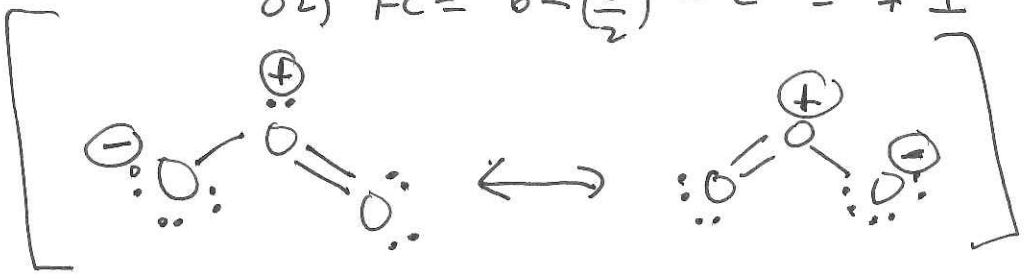
Ozone =



↙ in stratosphere absorbs harmful UV rad.

O1) $FC = 6 - \left(\frac{2}{2}\right) - 6 = -1$

O2) $FC = 6 - \left(\frac{6}{2}\right) - 2 = +1$



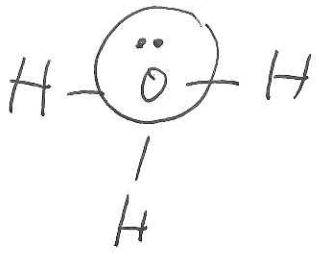
Resonance structures often have formal charges associated with them.

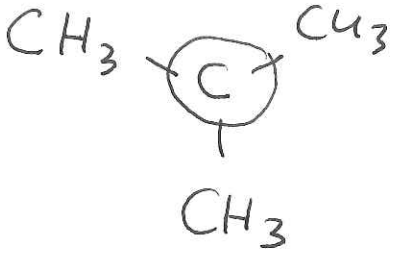
— resonance indicated by double-headed arrow

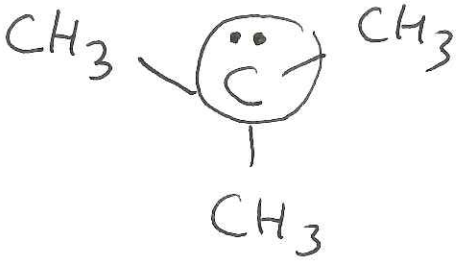
— only diff is placement of π + non-bonding valence e^-s] connections btwn atoms the same

Problems for home

4

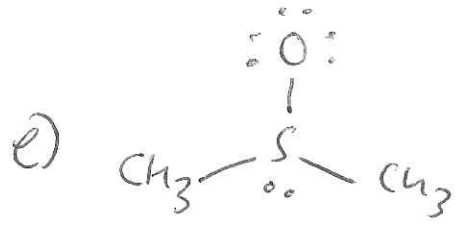
a) 

b) 

c) 

d) 

methyl isocyanide

e) 

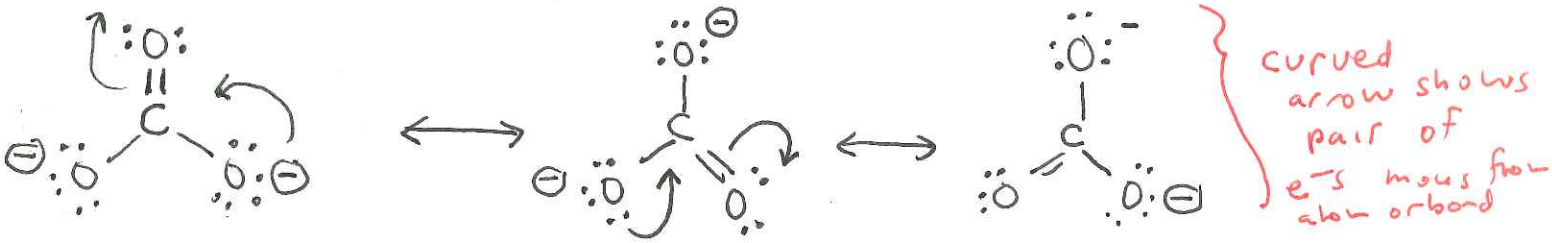
Calculate Formal charges for the circled atom

Resonance

- Lewis structures have a problem in that they impose an artificial location for the e^-s.
- More than one equivalent Lewis structure can be written for many molecules or ions

e.g. CO_3^{-2} (carbonate)

repr. movement of 2 e^-s

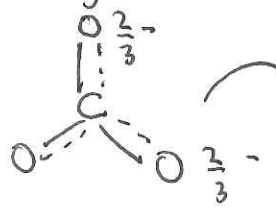


- We call the ~~3~~ "resonance structures" — differ only in placement of π or nonbonding e^-s
- Connected by double-headed arrows to indicate that the actual molecule or ion will be represented by a hybrid of these structures (not ⇌ (rapid equilibrium) of valence isomers)

C-O Bond order = 1.33

Actual structure of carbonate may look like the following non-Lewis structure

{ more stable than any indiv. resonance form }



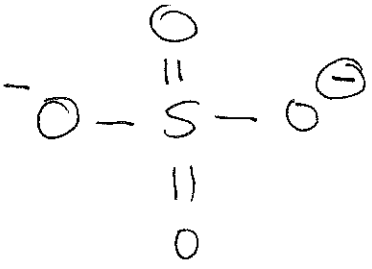
resonance hybrid

dashed line = delocalized e^-s

Take home problem

Draw all resonance (Lewis dot) structures of the sulfate ion:

SO_4^{-2}



In CO_3^{-2}, bonds are all 1.28 A°

C–O single bond ~ 1.43 A°

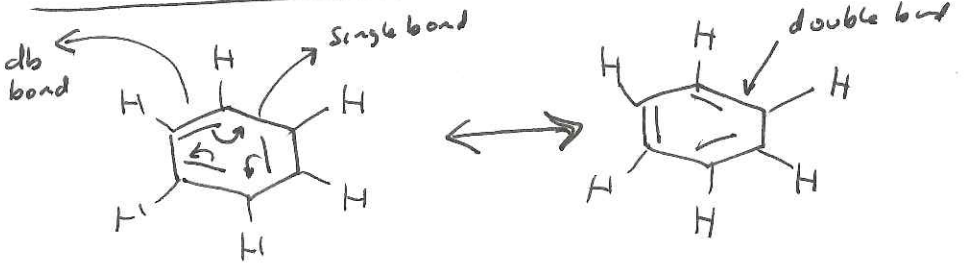
C=O double bond 1.20 A°

1 A° = [redacted] =

10^{-10} m

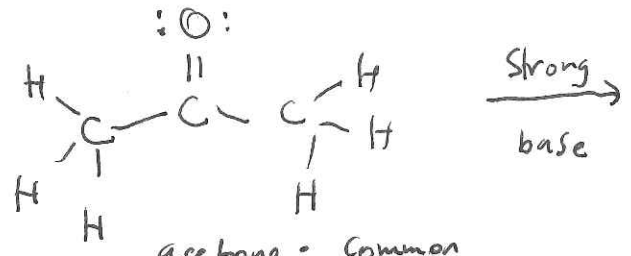
= 100 pm

Resonance in aromatic systems:

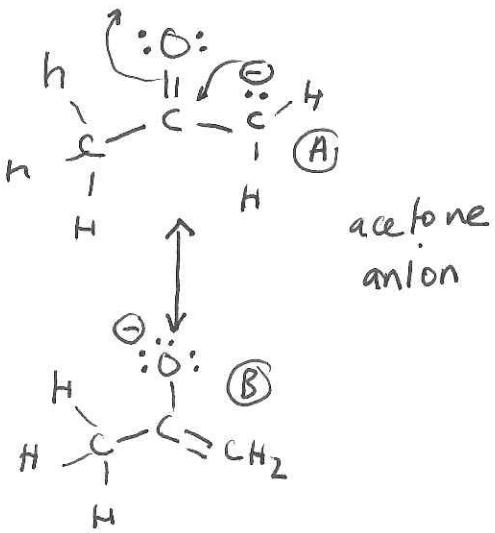


(ppt slide)

However, different resonance structures of a molecule don't have to be equivalent:



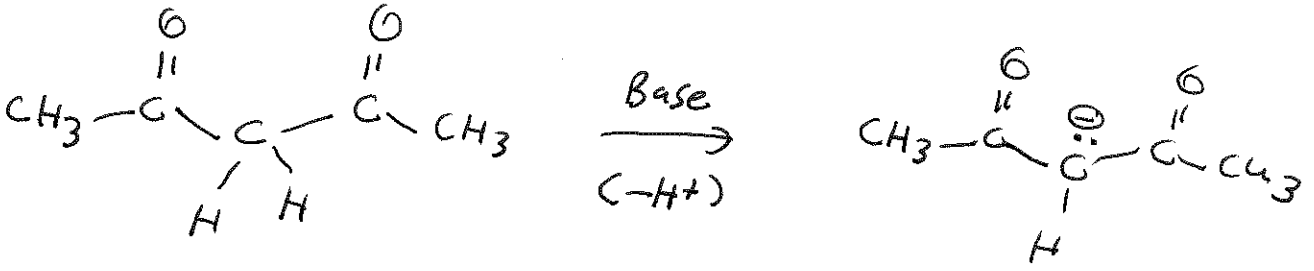
acetone: common solvent



In this case, the actual structure of the resonance hybrid is closer to the more stable form (B)

(places negative chg on more EN oxygen atom)

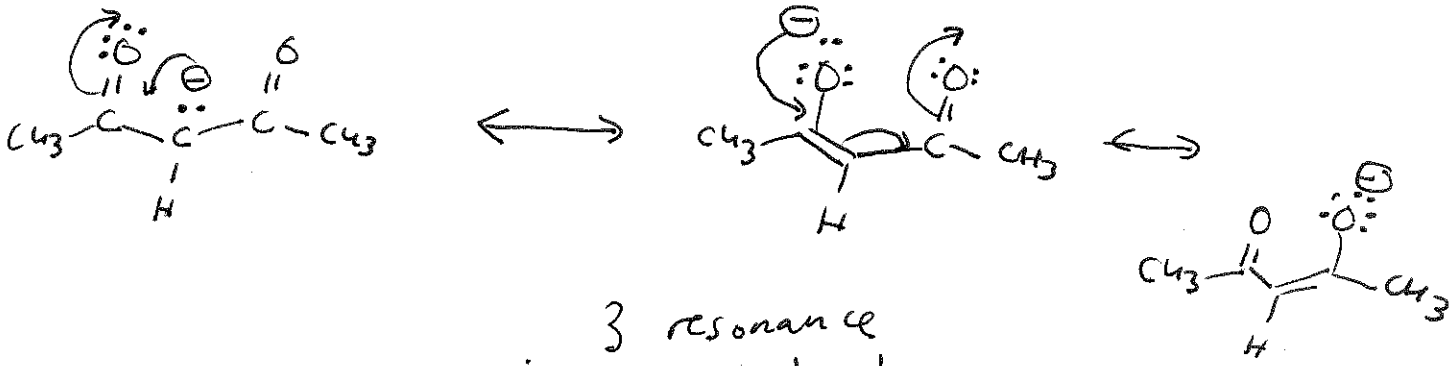
A slightly more complex example:



2,4-pentanedione

2,4-pentadione ion

Formal (−) charge on central C.



3 resonance structures result from e⁻ delocalization

(2.7)

Acid - Base Chemistry

concept related to electronegativity + polarity

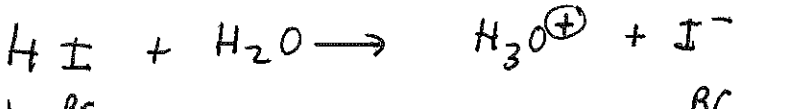
Bronsted - Lowry theory

1) Acid: substance that can donate (or lose) a proton (H^+)

2) Base: substance that can accept (or remove) a H^+

H^+ acceptor — H^+ donor — conj. acid of H_2O — conj. base of HCl

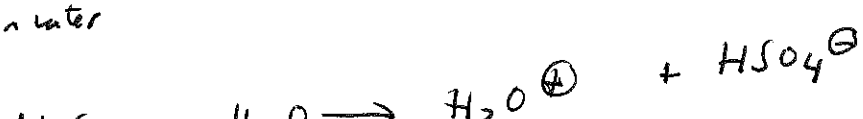
(H_3O^+) hydronium ion

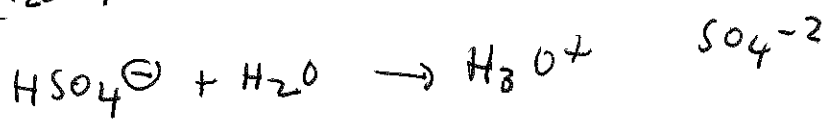


completely transfer H^+ in water

Bronsted acid → donate hyd. ion (H^+)

Bronsted base → accepts H^+





Sulfuric acid has 2 protons it can transfer to a base (diprotic)

Strength of acids & bases:

K_a and pK_a

In contrast to HCl & H_2SO_4, AcOH (vinegar) is a much weaker acid:

* For 0.1 M AcOH (25°C), only 1% of AcOH ionize. by transferring their protons to H_2O

$$HA + H_2O \rightleftharpoons A^{\ominus} + H_3O^{\oplus}$$

$$K_{eq} = \frac{[H_3O^+]\,[A^-]}{[HA]\,[H_2O]}$$

$[H_2O]$ ess. const at 55.5 M

$$K_a = K_{eq}[H_2O] = \frac{[H_3O^+]\,[A^-]}{[HA]}$$

K_a ← acidity constant

At 25°C, acidic constant for AcOH = 1.76×10^{-5}

Typically express K_a as negative log: pK_a

$$pK_a = -\log K_a$$

$$pK_a = -\log(1.76 \times 10^{-5}) = 4.75$$