Water Analysis using field kits

7rd-12th September 2014 at MRRD

Chemical calculations

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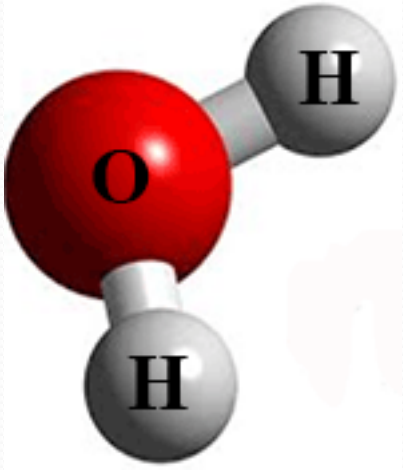
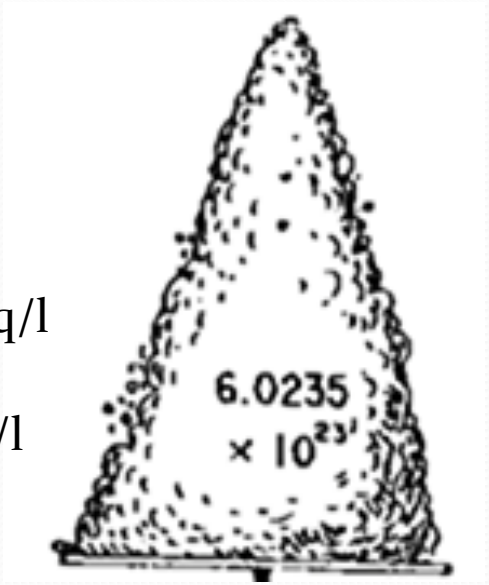


meq/l

mg/l



Project in MRRD covering Capacity Building and Institutional Cooperation in the field of Hydrogeology for Faryab Province Afghanistan

Milliequivalentse

Mole

NORPLAN

Why this topic - chemistry?

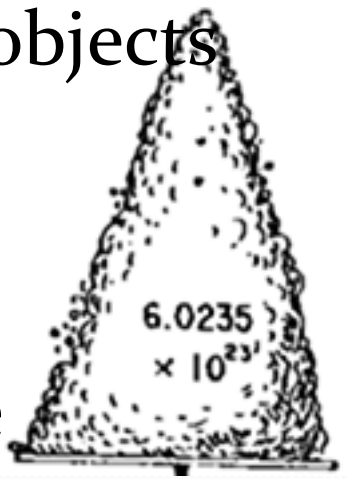
- *Preparing accurate reports of water analysis is important.*
- *Wrong units may cause wrong conclusion and wrong action.*

- *We will cover:*
  - *Calculation of mole and molarity*
  - *Units as mg/l*
  - *Conversions to milliequivalents - meq / liter*
  - *Calculation of pH*
  - *Calculation of alkalinity as mg/l of $CaCO_3$ or mmeqv/l*

Definitions – Mole

- Mole: SI unit of the amount of a substance
- This number is called Avogadro's number and is given by 6.022×10^{23}
- The mole is *NOT* just a counting unit, like the dozen, which specifies only the number of objects. The definition of a mole specifies the number of objects in a *fixed mass* of substance.

Definition: A mole is the number of atoms in exactly 12g of the carbon-12 isotope



One mole

Many, many atoms or molecules in a Mole!!!

6 022 000 000 000 000 000 000 000

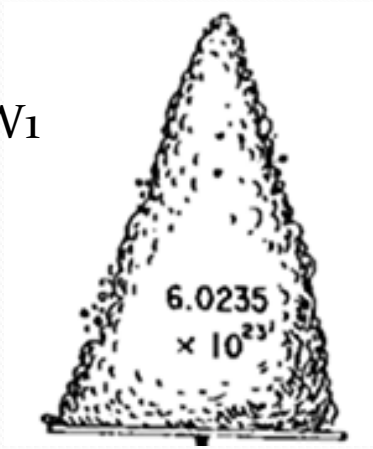
Or 6.022×10^{23}

- So we can also calculate the weight of one atom of molecule if we want ☺

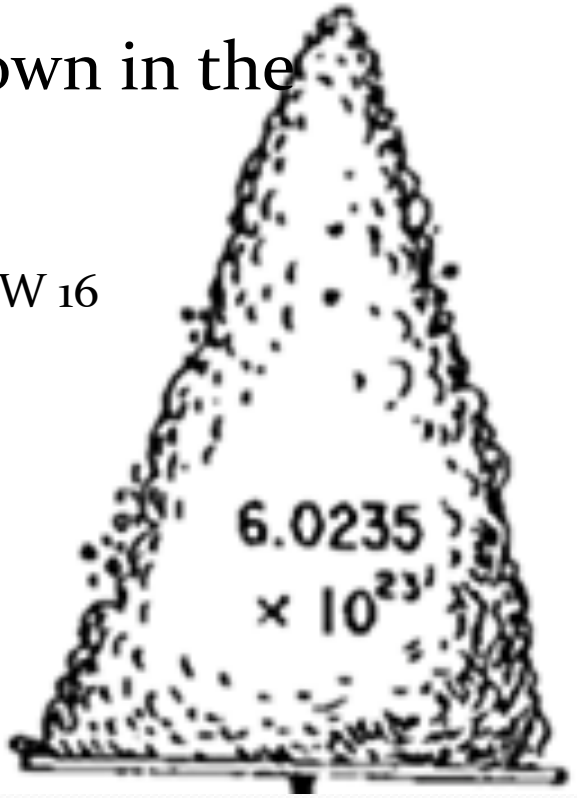
Mole exampe for water

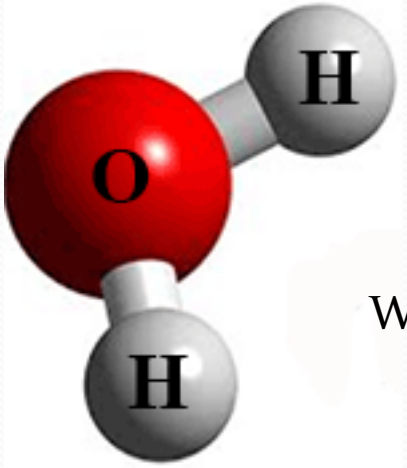
- The gram weight of 1 mole of atoms as shown in the periodic table.

2 mole hydrogen MW1



I mole Oxygen MW 16





Water = H_2O = $2H^+ + O^{2-}$

Or 2 mol H reacts with 1 mol O

Why is mole important

- Because in chemistry we work with amount of atoms, molecules in differernt forms. Rather than talking in number of molecules, or atoms, we talk in terms of moles or millimoles. Much easier.

- We need this to balance equations, like how many atoms or one compound react with another compound.

- $NaOH + HCl = NaCl + H_2O$
- (balance moles and work out weight of each..?)

Periodic table:

Period																	
1	1 H 1.008																2 He 4.003
2	3 Li 6.94	4 Be 9.012											5 B 10.81	6 C 12.01	7 N 14.01	8 O 16.00	9 F 19.00	10 Ne 20.18
3	11 Na 22.99	12 Mg 24.31											13 Al 26.98	14 Si 28.09	15 P 30.97	16 S 32.06	17 Cl 35.45	18 Ar 39.95
4	19 K 39.10	20 Ca 40.08	21 Sc 44.96	22 Ti 47.88	23 V 50.94	24 Cr 52.00	25 Mn 54.94	26 Fe 55.85	27 Co 58.93	28 Ni 58.69	29 Cu 63.55	30 Zn 65.39	31 Ga 69.72	32 Ge 72.64	33 As 74.92	34 Se 78.96	35 Br 79.90	36 Kr 83.79
5	37 Rb 85.47	38 Sr 87.62	39 Y 88.92	40 Zr 91.22	41 Nb 92.91	42 Mo 95.96	43 Tc (98)	44 Ru 101.1	45 Rh 102.9	46 Pd 106.4	47 Ag 107.9	48 Cd 112.4	49 In 114.8	50 Sn 118.7	51 Sb 121.8	52 Te 127.6	53 I 126.9	54 Xe 131.3
6	55 Cs 132.9	56 Ba 137.3	*	72 Hf 178.5	73 Ta 180.9	74 W 183.9	75 Re 186.2	76 Os 190.2	77 Ir 192.2	78 Pt 195.1	79 Au 197.0	80 Hg 200.5	81 Tl 204.38	82 Pb 207.2	83 Bi 209.0	84 Po (209)	85 At (210)	86 Rn (222)
7	87 Fr (223)	88 Ra (226)	**	104 Rf (265)	105 Db (268)	106 Sg (271)	107 Bh (270)	108 Hs (277)	109 Mt (276)	110 Ds (281)	111 Rg (280)	112 Cn (285)	113 Uut (284)	114 Fl (289)	115 Uup (288)	116 Lv (293)	117 Uus (294)	118 Uuo (294)

Lanthanide Series*	57 La 138.9	58 Ce 140.1	59 Pr 140.9	60 Nd 144.2	61 Pm (145)	62 Sm 150.4	63 Eu 152.0	64 Gd 157.2	65 Tb 158.9	66 Dy 162.5	67 Ho 164.9	68 Er 167.3	69 Tm 168.9	70 Yb 173.0	71 Lu 175.0
Actinide Series**	89 Ac (227)	90 Th 232	91 Pa 231	92 U 238	93 Np (237)	94 Pu (244)	95 Am (243)	96 Cm (247)	97 Bk (247)	98 Cf (251)	99 Es (252)	100 Fm (257)	101 Md (258)	102 No (259)	103 Lr (262)

How to read the periodic table?

- *What is the weight of an atom?*
- *- Calsium?*
- *- Calcium Carbonate (CO_3)*

- *Lets look at the table and calculate:*
- A mole is that quantity of a substance whose mass in grams is the same as its formula weight
- E.g. Fe55.85
- Iron has an atomic mass or 55.85g mol^{-1}, so one mole of iron has a mass or 55.85g

What is molarity?

- Mole is just particles
- But in solution like water? We use Molarity
- Molarity is the number of moles of solute in 1 Litre (L) of solution

- M = Molarity = no. of moles
- volume in Litres

Example to calculate molarity

Milliequivalents Definition

- mEq = represents the amount in milligram, of a solute equal to 1/1000 of its gram equivalent weight taking into account valence of ion

$$\text{Eq weight (g)} = \frac{g\ atomic\ or\ molecular\ weight}{valence}$$

mEq as number of units = mmol/valency

Milliequivalents

- Meq is related to the chemical activity of an electrolyte
- It is related to the total number of ionic charges in solution and considers the valence (charge of each ion)
- For any given chemical compound the milliequvalents of cations equals that of anions
- Example:
  - a solution of NaCl will contain the same number of milliequivalents of Na+ (the cation) as it will Cl- (the anion).
- For compounds with valency of 1 mmol = meqv

Eq for mono-, di- and tri- valent ions

- For monovalent ions, 1 meq = 1 mmol
- For divalent ions, 1 meq = 0.5 mmol
- For trivalent ions, 1 meq » 0.333 mmol

Example

Example calculate molarity

What is molarity of an 85.0mL ethanol (C_2H_5OH) solution containing 1.77g of ethanol?

Step 1: Determine the number of moles of ethanol

Molar mass of ethanol, C_2H_5OH:

2 × carbon atoms	2 × 12.01 $gmol^{-1}$	24.02 $gmol^{-1}$
1 × oxygen atom	1 × 16.00 $gmol^{-1}$	16.00 $gmol^{-1}$
6 × hydrogen atoms	6 × 1.008 $gmol^{-1}$	6.048 $gmol^{-1}$
		46.07 $gmol^{-1}$

$$\text{No. of moles} = \frac{\text{mass in g}}{\text{molar mass}}$$

$$\text{No. of moles ethanol} = \frac{1.77\text{g}}{46.07\ gmol^{-1}} = 0.038\ \text{mol}$$

Step 2: Convert to molarity

Have 85.0mL ethanol

1 L = 1000mL

⇒ Have 0.085 L of ethanol

$$\text{Molarity} = \frac{\text{no. of moles}}{\text{volume in L}} = \frac{0.038\ \text{mol}}{0.085\ \text{L}} = 0.45\ \text{mol L}^{-1} \equiv 0.45\ \text{M}$$

Questions

Calculate the molarities of each of the following solutions:

(a) 2.357g of sodium chloride (NaCl) in 75mL solution

Answer: 0.5378 M

(b) 1.567mol of silver nitrate ($AgNO_3$) in 250mL solution

Answer: 6.268 M

(c) 10.4g of calcium chloride ($CaCl_2$) in 2.20×10^2 mL of solution

Answer: 0.426 M

Lets go further to eqvivalents

- Mole = Avogadros's mumber (6.023 x 10E23)
- Molecular weight (MW) = weight in grams of one mole
- Millimole = 1/1000 mole
- Valence= Amount of charge of an ion
- Equivalents (Eq) = number of univalent counter ions needed to react with each molecule of substance (in moles)

- Example HCA has equivalent of 1 per mole in that mole of H+ reacts with one mole of Cl-

Calculations with Milli equivalents

- Converting milliequvalents to weights
- Converting weights to milliequivalents
- Converting mg% to mEq/l

- For monovalent ions, 1 meq = 1 mmol
- For divalent ions, 1 meq = 0.5 mmol
- For trivalent ions, 1 meq » 0.333 mmol

meq = mmol/vanency

- 1. How many equivalents are present in 80 grams of calcium (molecular weight » 40 g)?
- 2. How many equivalents of sodium are present in 116 g of NaCl (molecular weight of Na » 23; molecular weight of Cl » 35)?
- 3. How many millimoles of Mg^{+2} would be present in a solution containing 0.8 milliequivalents?
- 4. How many milliequivalents of P^{-3} are present in a solution containing 6 millimoles?

Listing of Atomic Weights, Valences, and Equivalent Weights for Common Ions

	Atomic/Formula Weight	Valence	Equiv Wt (Atomic/valence)
Al^{+++}	27	3	9
NH_4^+	18	1	18
Ca^{++}	40	2	20
Fe^{+++}	56	3	18.7
Mg^{++}	24	2	12
K^+	39	1	39
Na^+	23	1	23
$C_2H_30_3^-$	59	1	59
$HC0_3^-$	61	1	61
$C0_3^{--}$	60	2	30
Cl^-	35.5	1	35.5
$S0_4^-$	96	2	48

Convert between mole and mass

- Mole is number of particles or atoms.
- To convert to mass (kg, g, mg etc) we have first to find the molar weight. This we find from the periodic table.

- 1 mole of water weights $2H + O = 2 \times 1 + 16 = 18$ g

- Mass = n moles x mole weight
- Mass of n moles of H_2O = n x Mole Wt(g)

- So 5 moles of water has a mass of $5 \times 18 = 90$ g

Calculation examples

- What is the concentration of a solution containing 4 mEq/l of KCl?
  - Step 1
    - Molecular weight of KCl :
      - Molecular weight of Potassium (K) = 39
      - Molecular weight of Chloride = 35.5
      - MW of KCl = 39 + 35.5 = 74.7 g

Calculation cont- meqv

- Step 2: Calculate equivalent weight.
  - Equivalent weight= molecular weight / valence
  - Since valence of KCl = 1, Equiv. wt = 74.5 g

- Step 3:
  - 1 mEqv KCl = 1/1000 x 74.5 g= 0.0745g = 74.5mg

- Step 4: 4 x mEqv/l of KCL = 4 x 74.5 mg = 298 mg/l

pH

- $H_2O \leftrightarrow H^+ + OH^-$
- $pH = -\log_{10}[H^+]$
- $(H) = 10^{-pH}$
- Example What is the concentration of H in solution of pH = 2.5?
- Answer: $10(-2.5) = 10^{-0.5} \times 10^{-2}$
- $= 1/3.16 \times 10^{-2} = 0.31 \times 10^{-2}$ mol/l

Expressing nitrate and phosphate

- Express 10 mg/ NO_3 as N?
- Express 10 mg NO_3 as meqv?

Calculation: Step 1 Calculate mw of NO_3

Nitrogen	=	14.01	14.01
3 x oxygen	=	3 x 16 =	48.03
MW of NO_3 =			62.04

mole? 10 mg/62.04 mg/mmole = 0.161 mmole

10 mg/l NO_3 = 14.01 x 0.161 = 2.25 mg/l NO_3 as N

Calculate Nitrate as mEqv

- Step 1 convert 10 mg/l NO_3 as NO_3 to meqv/l
  - Eqv wt = atomic wt or molecular wt/ valence
  - Valence of NO_3 = 1. (As in HNO_3 , nitric acid)
  - $H^+ + NO_3^-$ (Valence =1)
  - Eqv wt = 62.04/1 for NO_3
  - Eqw = mol. x eqv wt = 0.161 x 62.04 = 10mg/l as NO_3

Calculate PO4

- What is 25 mg/l phosphate as P expressed as meqv/ l
- Or expressed as P?

- Lets do the calculation together.

Alkalinity calculations

- **Phenolphthalein Alkalinity to pH 8.3**
- $CO^{32-} + H^{+} \rightarrow ?HCO^{3-}$

- **Total alkalinity to pH 4.3**
- $HCO^{3-} + H^{+} \rightarrow ?H^{2}CO^{3}$

OH^-	Hydroxide ion (base)
H_2CO_3	Carbonic acid
HCO_3^-	Bicarbonate ion
CO_3^{2-}	Carbonate ion
$CaCO_3$	Calcium carbonate (calcite)
$CaMg(CO_3)_2$	Dolomite lime

Alkalinity calculations

- **Phenolphthalein Alkalinity**
- Ex. 2.0ml of 0.01M of sulfuric acid was required to titrate 50ml of your sample to pH 8.3. What is the alcalinity

- **Total Alkalinity**
- Ex. 18.0ml of 0.01M of sulfuric acid was required to titrate 50ml of your sample to pH 4.5.

What is the Alkalinity as meq and as mg $CaCO_3$?

Result Alkalinity calc.

- pH8.3:
  - Acid used: 2 ml per 50 ml = 40 ml/l
  - Mole: 0.040l x 0.01M/l = 0.0004 mole of H_2SO_4
    - = 0.0008 eq = 0.8 meq
    - Expressed as $CaCO_3$: MW = 100.09 g /mole
      - = 50.05 g/eq
    - = 0.8 meq x 50.05 mg/meq = 360 mg /l $CaCO_3$

Cation – anion balance

- In a solution cations and anions always balance

- Which unit do we use for checking balances?

Example Cation- Anion balance

Cation- Anion Balance:

	Formula	wt	Valence	mg/l	meq/mg	meq/l
Bicarbonate	HCO3	128	1		61	0.00
Sulphate	SO4	2	2		48	0.00
Chloride	Cl	1274	1		35.5	0.00
				Sum		0.00
Calsium	Ca	86	2		20.04	0.00
Mangnesium	Mg	21	2		12.16	0.00
Potassium	K	7.7	1		39.1	0.00
Sodium	Na	1392	1		23	0.00
				Sum		0.00
				% Out of balance:		#DIV/0!

Example complete balance

- Anions:

Cation- Anion Balance:

	Formula	wt	Valence	mg/l	meq/mg	meq/l
Bicarbonate	HCO3	61	1	248	61	4.07
Sulphate	SO4	80	2	690	48	14.38
Chloride	Cl	35.5	1	985	35.5	27.75
				Sum		46.19
Calsium	Ca	40.08	2	250	20.04	12.48
Mangnesium	Mg	24.3	2	22	12.16	1.81
Potassium	K	39.1	1	14	39.1	0.36
Sodium	Na	23	1	820	23	35.65
				Sum		50.29
				% Out of balance:		8.17%

Thank you

- Hope you have enjoyed some of this . You will find all supporting examples on the web.