ICP ANALYTICAL RESULT COMPUTATIONS

STEP 1: COMPUTING LOI

Measurements / computations needed:

1. Weight of ceramic boat ($\mathbf{m_{cb}}$)
2. Before weight of sample ($\mathbf{m_{sb}}$)
3. Mass of sample & boat after ignition ($\mathbf{M_{sample\&boat}}$)

Calculations:

Mass BEFORE LOI: $\mathbf{m_{sb}}$

Mass AFTER LOI: $\mathbf{m_{sa}} = \mathbf{M}_{\text{sample\&boat}} - \mathbf{m_{cb}}$

LOI CALCULATION: $$LOI\% = 100 - \left(\frac{m_{sa}}{m_{sb}} \times 100\right)$$

Example:

$m_{cb} = 6.3382$g $m_{sb} = 1.0514$g $M_{sample\&boat} = 7.3367$g

$$LOI\% = 100 - \left(\frac{(7.3367g - 6.3382g)}{1.0514g} \times 100\right) = 5.0313\%$$

LOI remaining sample (rs) expressed as a decimal = 1- 0.050313 = **0.949687**

STEP 2: PREPARING THE ICP RESULTS FOR COMPUTATION

2.1 Subtract the “BLANK” results from your sample results. Results with a “negative” sign are recorded as ZERO!

2.2 Remove “nonsensical” results; e.g. Li & B - from our Lithium Borate flux, N & Cl - from the aqua regia, Ar - from the Argon plasma gas, etc.

2.3 Convert all remaining results to PPM if necessary. All your data should be in ppm.

STEP 3: COMPUTING THE ELEMENTAL CONCENTRATIONS IN YOUR ACTUAL DRY ROCK , MINERAL, or SOIL SAMPLE

Measurements needed:

1. I_{ms} = ICP instrument read out MINUS blank in PPM as computed in STEP 2
2. df = dilution factor of the final sample processed through the ICP (1000x: $0.1\,mL_{AquaRegiaDigest}$ filled to 100mL w/ DI H_2O)
3. m_a = mass of the Aqua Regia used that received the borax flux melt in grams (g)
4. m_{bf} = mass of borate flux used in grams (g)
5. m_s = mass of the dry sample powder used in grams (g)

$$C_{element} = I_{ms}(ppm) * \frac{m_a + m_{bf}}{m_s} \times df$$

FUSION DIGESTION CALCULATIONS

$C_{element}$ = element concentration in the solid

Example:
m_s = 0.2285g mb_f = 1.3284g m_a = 102.56g df = 1000
I_{ms} ICP analytical instrument reading minus “Blank” in ppm = 0.346 ppm

$C_{element}$ = 0.346 ppm × (102.56g + 1.3284g) / 0.2285g × 1000 = 157,310 ppm
Round answer to appropriate sig.digs based on PPM reported by the instrument, example here: 157,000 ppm

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STEP 4: CONVERT PPM TO % FOR ROCK / MINERAL FORMING OXIDES

The rock forming oxides are SiO_2, Al_2O_3, FeO or Fe_2O_3, CaO, MgO, Na_2O, K_2O, TiO_2, P_2O_5. Results for these oxides are reported as PERCENT. All other elements analyzed are reported as elements and in PPM.

Convert the $C_{element}$ computed in STEP 3 into the correct oxide % for oxides listed:

$$Oxide(\%) = C_{element}(ppm) \times \frac{AMU_{oxide}}{AMU_{element}} \times 0.0001$$

Example:

$C_{element}$(ppm) = 157,000 ppm (as calculated in STEP 3 above)

Let's assume the measured element was Si $AMU_{Si} = 28.086$ $AMU_{SiO2} = 60.084$

$SiO_2\% = 157{,}000 \times 60.084 / 28.086 \times 0.0001 = 33.6\%_{SiO2}$

STEP 5: ERROR ANALYSIS & CORRECTION FOR OXIDES

All computed OXIDE PERCENTAGES together with the measured LOI PERCENTAGE should add up close to 100%. Note: For % of Iron Oxide use either FeO or Fe_2O_3! Do NOT use both when adding your percentages together.

If your result is close to 100% (± 3%), your analytical values are most likely correct. If not, and you are significantly off, then there is an error in your analysis. The most likely culprit is SiO_2. If all else fails you can allot the % deviation from 100% to SiO_2. Not great to be reporting analytical results, but this is likely the most correct estimation of the true SiO_2 value, unless some other oxides have also erroneous values.

You may also try "curving" your oxide percentages if the sum of all oxide % plus LOI is well over 100%.

1. Your LOI is probably correct. Therefore subtract LOI % from 100%. Example: LOI 5.6%; 100% - 5.6% = 94.4%. This value is your ADJUSTED SUM for "curving"!
2. Add up all your oxide % without LOI. Example: Oxide % sum without LOI = 148.3%. This is your RAW SUM value!
3. "Correct" each oxide percent by ***%oxide* × *ADJUSTED SUM* ÷ *RAW SUM***. Example: Al_2O_3 26.7%; 26.7 × 94.4 ÷ 148.3 = 16.9% corrected Al_2O_3 ! Do this for ALL oxides.
4. The sum of ALL **corrected** oxides plus the original LOI should now equal 100%.

Note: Be aware that if you are analyzing different materials, like ore minerals, you will show a significant error in the sum of usual oxide percentages. This error can be mitigated by calculating the oxides of these ore target elements (e.g. Cu, Zn, Pb, etc.- not included in the list of common oxides) and adding these to your percent summation together with the usual oxides.

Analytical Value Comparison:

How do your values compare? Check to see if your oxide composition approximate those of minerals, rocks or soil

Oxide Composition of Minerals

In order to assess oxide composition in minerals, go to **Webmineral.com**. Search a suspected mineral and open the Mineral Data link, usually #1 on the listing. The General Information for the mineral has a breakdown of the elemental composition as well as **Percent Concentration of Oxides** ! Compare these listed values with your analytical values for a suspected mineral and see how well these might correspond.

Oxide Composition of Common Igneous Rocks

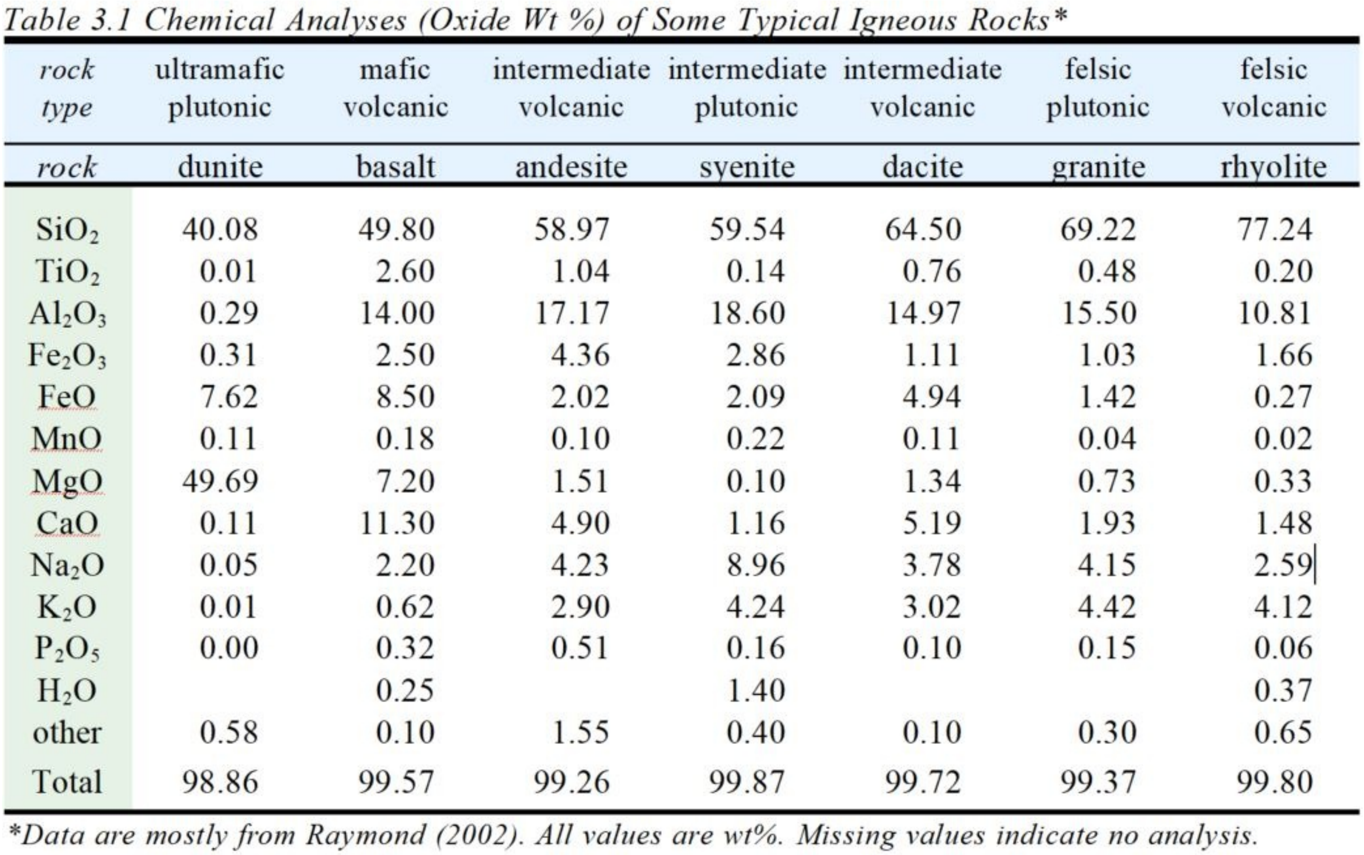
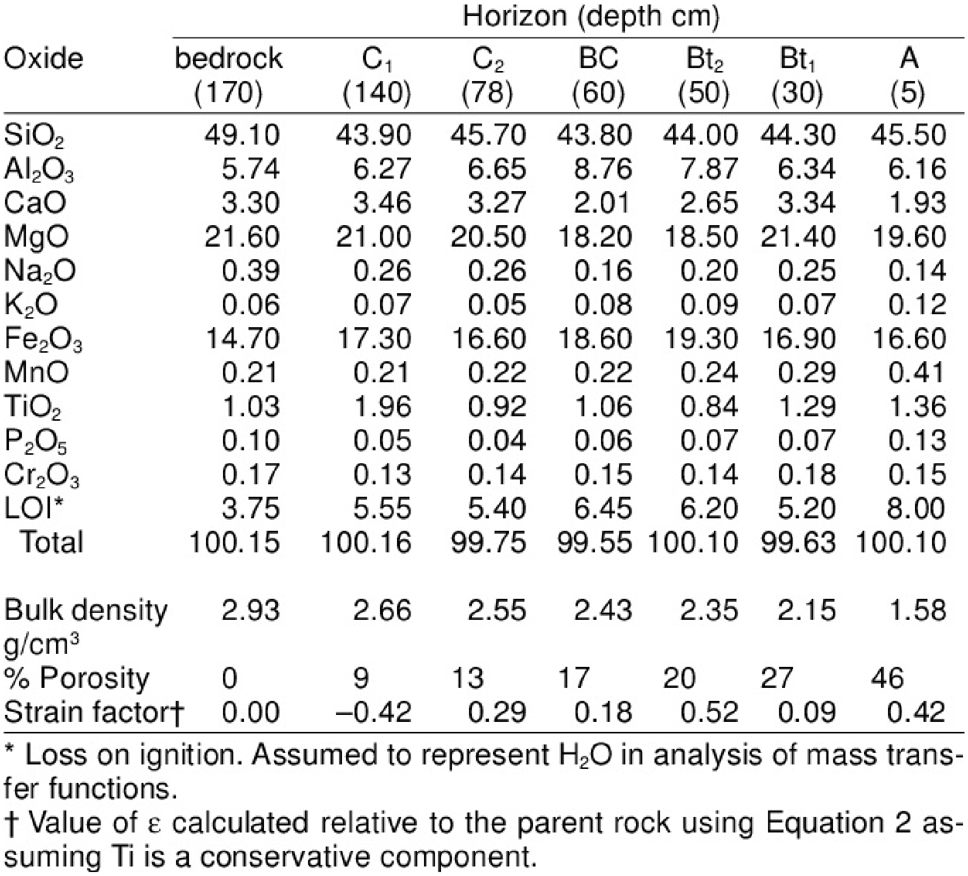


*Table 3.1 Chemical Analyses (Oxide Wt %) of Some Typical Igneous Rocks**

rock type	ultramafic plutonic	mafic volcanic	intermediate volcanic	intermediate plutonic	intermediate volcanic	felsic plutonic	felsic volcanic
rock	dunite	basalt	andesite	syenite	dacite	granite	rhyolite
SiO_2	40.08	49.80	58.97	59.54	64.50	69.22	77.24
TiO_2	0.01	2.60	1.04	0.14	0.76	0.48	0.20
Al_2O_3	0.29	14.00	17.17	18.60	14.97	15.50	10.81
Fe_2O_3	0.31	2.50	4.36	2.86	1.11	1.03	1.66
FeO	7.62	8.50	2.02	2.09	4.94	1.42	0.27
MnO	0.11	0.18	0.10	0.22	0.11	0.04	0.02
MgO	49.69	7.20	1.51	0.10	1.34	0.73	0.33
CaO	0.11	11.30	4.90	1.16	5.19	1.93	1.48
Na_2O	0.05	2.20	4.23	8.96	3.78	4.15	2.59
K_2O	0.01	0.62	2.90	4.24	3.02	4.42	4.12
P_2O_5	0.00	0.32	0.51	0.16	0.10	0.15	0.06
H_2O		0.25		1.40			0.37
other	0.58	0.10	1.55	0.40	0.10	0.30	0.65
Total	98.86	99.57	99.26	99.87	99.72	99.37	99.80

**Data are mostly from Raymond (2002). All values are wt%. Missing values indicate no analysis.*

Oxide Composition of Soils



	Horizon (depth cm)						
Oxide	bedrock (170)	C_1 (140)	C_2 (78)	BC (60)	Bt_2 (50)	Bt_1 (30)	A (5)
SiO_2	49.10	43.90	45.70	43.80	44.00	44.30	45.50
Al_2O_3	5.74	6.27	6.65	8.76	7.87	6.34	6.16
CaO	3.30	3.46	3.27	2.01	2.65	3.34	1.93
MgO	21.60	21.00	20.50	18.20	18.50	21.40	19.60
Na_2O	0.39	0.26	0.26	0.16	0.20	0.25	0.14
K_2O	0.06	0.07	0.05	0.08	0.09	0.07	0.12
Fe_2O_3	14.70	17.30	16.60	18.60	19.30	16.90	16.60
MnO	0.21	0.21	0.22	0.22	0.24	0.29	0.41
TiO_2	1.03	1.96	0.92	1.06	0.84	1.29	1.36
P_2O_5	0.10	0.05	0.04	0.06	0.07	0.07	0.13
Cr_2O_3	0.17	0.13	0.14	0.15	0.14	0.18	0.15
LOI*	3.75	5.55	5.40	6.45	6.20	5.20	8.00
Total	100.15	100.16	99.75	99.55	100.10	99.63	100.10
Bulk density g/cm^3	2.93	2.66	2.55	2.43	2.35	2.15	1.58
% Porosity	0	9	13	17	20	27	46
Strain factor†	0.00	–0.42	0.29	0.18	0.52	0.09	0.42

* Loss on ignition. Assumed to represent H_2O in analysis of mass transfer functions.

† Value of ε calculated relative to the parent rock using Equation 2 assuming Ti is a conservative component.