

Principle of Electroneutrality

Purpose: The purpose of this assignment is to learn how to determine whether all major inorganic constituents have been determined in Lithia water by applying the principle of electroneutrality.

Learning Outcomes: At the end of this assignment, students will be able to:

1. Apply the principle of electroneutrality toward calculating cation and anion concentrations in natural waters
2. Understand the purpose of univariate statistical tests in comparing concentrations of ionic solutes
3. Perform appropriate chemical and statistical calculations for the comparison of ionic solute populations.

Preparation: To ensure that each student has received a proper introduction to the statistical fundamentals of chemical analysis problems, everyone will complete a laboratory exercise using the following ASDL resource:

1. Harvey, D.; Otto, W. Introduction to Data Analysis. *JASDL* [Online], **2007**, article 10042. <http://asdl.org/onlineArticles/ecourseware/Harvey/DataAnalysisHome.html> (accessed November 29, 2013).

The use of univariate statistics is critical in evaluating the results of chemical determinations. In addition to completing the ASDL laboratory exercise entitled "Introduction to Data Analysis," to review basic statistical methods and measures of accuracy and precision, students should also read Chapter 4, "Evaluating Analytical Data," in David Harvey's textbook *Analytical Chemistry 2.0*, which is available at the Analytical Sciences Digital Library (ASDL) website (http://www.asdl.org/onlineArticles/ecourseware/Analytical_Chemistry_2.0/Welcome.html).

Characterization of Inorganic Ions in Lithia Water: Assessing whether the complete analysis of the major inorganic species in a Lithia water spring has been accomplished requires a statistical evaluation of the cation and anion concentrations determined in the sample. This assessment is based on the hypothesis that, using analytical techniques encountered in the traditional quantitative analysis laboratory, all detectable cations and anions have been determined. To test this hypothesis, one first must ask how the concentrations of all cationic and anionic species are related to one another in solution. Subsequently, one must then use this information to determine whether these two quantities, the concentration of cations in Lithia water and the concentration of anions in Lithia water, are statistically equivalent at a specified confidence level or whether there is a significant difference between the concentration of cations and anions determined in a Lithia water sample.

Lithia water, as with all matter, should follow the principle of electroneutrality, which states that all pure substances have no net charge. Remember that a solution, such as Lithia water, is simply a mixture of pure substances. Mathematically, one can express this principle in the following manner:

$$\sum_{i=1}^N n_{+} = \sum_{i=1}^N n_{-}$$
$$\sum_{i=1}^N c_{i,+} z_{i,+} = \sum_{i=1}^N c_{i,-} z_{i,-}$$

In the first equation above, n_{+} and n_{-} represent the moles of positive and negative charges, respectively. The moles of positive charge are calculated by multiplying the molarity of each cation ($c_{i,+}$) by the charge on each cation ($z_{i,+}$) and summing across all cationic charges. An identical calculation is performed to determine the moles of negative charge in a solution. This process is identical to writing a charge balance equation.

Q1. Once you have completed your Lithia water project experiments in lab, list the cations and anions that were determined. If you are performing these modules as part of a dry lab, please use the 1915 analysis plaque (Figure 2 – Major Inorganic Constituents in Statement of Problem module) to create your list of cations and anions.

Q2. Based on the principle of electroneutrality, what should be true about the concentration of the cationic and anionic charges in Lithia water?

Q3. Assuming that the inorganic constituents of Lithia water have been completely characterized, write down an appropriate charge balance equation for all dissolved ions in Lithia water.

Statistical Analysis of Electroneutrality:

Although solutions theoretically have equivalent concentrations of positive and negative charge, experimental error in the determination of solute concentrations will result in numerical differences between the total concentrations of cations and anions. Often times, it is unclear whether these concentration differences are real (aka **bias or determinate error**) or due to random (indeterminate) error. Assuming that the experimental error is normally distributed, Chapter 4 in *Analytical Chemistry 2.0* provides an overview of how to calculate the uncertainty of measured quantities and to compare the means of two populations to determine if they are statistically significant for a given confidence level.

Q4. Use the error propagation equations described in Chapter 4 of *Analytical Chemistry 2.0* to propagate the experimental error in the following analytical determinations

- a. A solution with a volume of 1.000 ± 0.012 mL was determined to have a mass of 1.008 ± 0.023 g. What is the density of the solution and its uncertainty?
- b. The volume delivered by a buret (ΔV) is the difference between the initial volume (V_i) and the final volume (V_f) read on the scale of the buret. If V_i is (5.36 ± 0.02) mL and V_f is (15.68 ± 0.02) mL, calculate the volume delivered and its uncertainty.
- c. The density of a liquid was determined by measuring the mass of a 100-mL volumetric flask filled with the liquid, subtracting the mass of the empty 100-mL volumetric flask, and dividing the mass difference by the volume of the 100-mL volumetric flask. If the mass of the full flask is 248.3 ± 0.1 g, the mass of the empty flask is 45.5 ± 0.1 g, and the volume of the flask is 100.0 ± 0.08 mL, calculate the density of the liquid and its uncertainty.

Q5. Based on your reading of Chapter 4 in *Analytical Chemistry 2.0*, what statistical approach would you use to determine whether equivalent amounts of cationic charge and anionic charge were determined in Lithia water?

Q6. The Nutrition Facts label on a bottle of local mineral water contains the following information for selected inorganic solutes (standard deviations provided by author, assume each result based on triplicate readings ($n=3$)):

Solute	Concentration (mg L^{-1})
Bicarbonate	466 (± 24)
Magnesium	124 (± 5)
Calcium	2.67 (± 0.10)
Sodium	3.31 (± 0.15)
Zinc	4.45 (± 0.10)

At the 95% confidence level, determine whether all of the major inorganic solutes have been reported on the Nutrition Facts label from this bottle of mineral water.