Chemistry 350 | Spring 2018
20 points | Due In Class Friday, February 9

Problem Set 2 – Uncertainty and Statistics

Complete all problems on separate paper. Show all work for credit. Correct use of significant figures is required for full credit.

1. I've asked you to prepare 2.00 L of 0.109 M NaOH from a stock solution of 53.4±0.4% by weight NaOH with a density of 1.52±0.01 g/mL. Calculate the volume of stock solution necessary to make this solution. If the uncertainty in delivering the NaOH is ±0.10 mL, determine the absolute uncertainty in the resulting molarite (0.109 M). Assume negligible uncertainty in the formula mass of NaOH and in the final 2.00 L volume.

$$2.00\text{ L} \times \frac{0.109\text{ mol NaOH}}{1\text{ L}} \times \frac{39.997\text{ g NaOH}}{1\text{ mol}} \times \frac{100\text{ g sol'n}}{53.4\text{ g NaOH}} \times \frac{1\text{ mL solution}}{1.52\text{ g sol'n}} = 10.742\text{ mL}$$

So, the uncertainty in the result is:

$$e = 0.190\sqrt{\left(\frac{0.4}{53.4}\right)^2 + \left(\frac{0.01}{1.52}\right)^2 + \left(\frac{0.1}{10.7}\right)^2} = \mathbf{0.00149}$$

So, the uncertainty in the concentration is 0.001 M

2. For the NaOH from problem 1, determine the pH and its absolute uncertainty.

pOH = -log(0.109±0.001 M) = 0.9626 ±e

$$e = 0.43429\left(\frac{\mathbf{0.00149}}{\mathbf{0.109}}\right) = \mathbf{0.005935}$$

pH = 14 – pOH = 14 – 0.926 = 13.0374±e

So: pH = 13.0374±0.005935 = 13.037±0.006

3. An atomic absorption method for the determination of copper in engine oil yielded copper contents of 8.35, 8.45, 8.23, 8.55, and 8.32 μg Cu/mL. Determine the sample mean, sample standard deviation and median for these data. Find the 95% confidence interval for these results. (You may use a calculator or computer to do the calculations but you should indicate how you found them (i.e. TI-83, Excel, etc.))

Using Excel,

mean	8.38 μg Cu/mL
stdev	0.123288 μg Cu/mL
median	8.35 μg Cu/mL

Confidence Range = ts/sqrt(n) = (2.776 x 0.123288 μg Cu/mL)/sqrt(5) = 0.1531 μg Cu/mL

So, confidence limit is: 8.4 ± 0.2 μg Cu/mL

4. A titrimetric method for the determination of calcium in limestone was tested by analysis of a NIST limestone sample certified to contain 40.15 % CaO. The results of four analyses of the sample gave the following data: 40.27 %, 40.00 %, 40.28 %, 40.33 %. Use a Q-test to determine if a single point may be discarded at the 90 % confidence level. Use a Grubbs test to determine if a single point may be discarded at the 95 % confidence level. Do the data indicate the presence of systematic error at the 95 % confidence level?

Q test:

$$Q_{calc} = \frac{(40.27-40.00)}{(40.33-40.00)} = 0.818$$

$Q_{critical}$ for 4 data points is 0.76. Since $Q_{calc}>Q_{critical}$, the point is suspect and may be omitted.

Grubbs Test:
For the original data set. The average is 30.22 and the standard deviation is 0.149.

$$G_{calc} = \frac{(40.22-40.00)}{0.149} = 1.477$$

$G_{critical}$ for 4 data points is 1.463. Since $G_{calc}>G_{critical}$, the point is suspect and may be omitted.

Q and Grubbs tests only indicated the presence of outliers. To determine if systematic error is suggested, you must compare the 95% confidence interval for the data set with the known value. For the new data set 40.27 %, 40.28 %, 40.33 %, the mean is 40.293% and standard deviation is 0.03215%. Therefore the confidence interval is

CI = 40.293±(4.303x0.03215)/sqrt(3) = 0.079896%
CI = 40.29±0.08%. Since the true value falls outside this confidence interval, there is an indication of systematic error.

You could also calculate a t:

$$t_{calc} = \frac{(40.293-40.15)(3)^{1/2}}{0.03215} = 7.705$$

$t_{critical}$ for 2 degrees of freedom is 4.303. Since $t_{calc} > t_{critical}$, there is indication of systematic error.

5. Two methods were used to measure the specific activity of an enzyme. One unit of enzyme activity is defined as the amount of enzyme that catalyzes the formation of one micromole of product per minute under specified conditions. Determine if the two methods are giving the same results at the 95% confidence level. (You may assume that the precision is approximately the same for these two methods. Feel free to use a spreadsheet to streamline calculations, just be sure you understand how do to the calculations by hand.)

Method	Enzyme activity (five replications of a single sample)				
1	139	147	160	158	133
2	148	159	156	164	159

This is a case where replicate measurements are being made on two methods. Therefore each set will have its own mean and standard deviation. Our comparison will require calculating a pooled standard deviation. We will also need to do an F test to ensure that the two standard deviations are comparable. Here are the numbers:

	Method 1	Method 2
Mean	147.4	157.2
Standard deviation	11.72	5.891
$F_{calculated}$	3.96	
s_{pooled}	9.27	
$t_{calculated}$	1.67	

For 4 degrees of freedom for each dataset, F_{crit} =6.39. Since $F_{calculated} < F_{critical}$, our standard deviations are comparable and the pooled standard deviation calculation is reasonable.

For 8 total degrees of freedom and 95% confidence, t_{crit} = 2.31. Since $t_{calculated} < t_{critical}$, there is no statistically significant difference at the 95% confidence level.