Using Confidence Limit Data to Evaluate Elemental Analysis

Now that you have analyzed the elemental makeup of your product, you want to use the data from the analysis to show that you have indeed synthesized the compound, $K_3[Fe(C_2O_4)_3]\bullet 3\ H_2O$. There is no way, by looking at the data, that we can know whether we did the experiment correctly. What we can do, however, is use the standard deviation to calculate confidence limits – a range within which the true value of the measured quantity should occur with a specified probability.

For a *large* number of measurements, the true value of x will be within the range x ± *s* for 68 per cent of the time, within the range x ± 1.96*s* for 95 per cent of the time. To be 99% certain that the correct answer is within a given range, we need to consider the range x ± 2.58*s*. In this experiment, we did not perform a "large" number of experiments, so we need to have some way of estimating our confidence for a smaller (less than infinite) number of experiments. To do this we introduce the variable, *t*. You can think of *t* as giving us some measure of the best we can do under the circumstances. Table 1 lists some factors that can be used for calculating confidence limits; as expected, these factors vary with n and the degree of confidence desired.

Table 1: Factors for Calculating Confidence Limits

Confidence Limit	**80%**	**90%**	**95%**	**99%**	**99.5%**
	$t/\sqrt{N}$	$t/\sqrt{N}$	$t/\sqrt{N}$	$t/\sqrt{N}$	$t/\sqrt{N}$
N					
2	2.17	4.46	8.98	45.0	450.
3	1.09	**1.69**	2.48	5.72	18.2
4	0.82	**1.18**	**1.59**	2.92	6.45
5	0.68	0.95	1.24	2.06	3.84
6	0.60	0.82	1.05	1.65	2.80
7	0.54	0.74	0.93	1.40	2.25
8	0.50	0.67	0.83	1.24	1.91
9	0.47	0.62	0.77	1.12	1.68
10	0.44	0.58	0.71	1.02	1.51

By using the expression:

$$\mu = \overline{X} \pm {}^{t}\!/\!_{\sqrt{N}} \bullet s$$

(where μ is the degree of confidence required, $\overline{X}$ is the mean, $t/\sqrt{N}$ is the confidence factor from Table 1, *N* is the number of replicates and s is the standard deviation) we generate a range of values.

For example, in determining the percentage of water in your compound, say you found that the mean percentage of water and standard deviation of your sample is 10.3 ±

0.6 % for 3 trials. To be 90% certain that the true value lies within our range of values, we can do the following calculation:

$$10.3\ \% \pm (1.69)(0.6\ \%) = 10.3 \pm 1.0$$

This means that you can be 90% sure that your experimentally determined value lies in the range between 9.3% - 11.3%.

You should now compare your experimentally determined percentage of water with the theoretical percentage of water in $K_3[Fe(C_2O_4)_3]\bullet 3\ H_2O$:

$$(3 \text{ mole } H_2O/1 \text{ mole } K_3[Fe(C_2O_4)_3]\bullet 3\ H_2O) \times 100\%$$
$$((3 \times 16.0 \text{ g/mole})/491.26 \text{ g/mole}) \times 100\ \% = 11.0\ \%$$

Since the theoretical percentage of water in $K_3[Fe(C_2O_4)_3]\bullet 3\ H_2O$ also lies in the range between 9.3% - 11.3% you can say that you **cannot** be sure at the 90% confidence limit that the experimental percentage is **different** than the theoretical percentage. (The 90 % or 95 % confidence limits are good choices for making these determinations). This is good – you are confident that there is no difference between experimental and theoretical percentage of water. This supports the idea that you did synthesize $K_3[Fe(C_2O_4)_3]\bullet 3\ H_2O$.

Let us look at another example, if the percentage of iron in a sample was found to be 10.5 ± 0.5 % for four trials. You can be 90% confident that the actual value will be in the range of 9.91% to 10.09% (10.5 % ± (1.18)(0.5)%). The theoretical percent of iron in $K_3[Fe(C_2O_4)_3]\bullet 3\ H_2O$ is 11.4 %. The theoretical value does not fall in the 90 % confidence limit range of your experimental data, in fact your experimental value appears to be lower than the theoretical value. You can say that you are 90 % confident that the percent iron is actually **lower** than the theoretically predicted amount.

You can increase the range of certainty for your experimentally determined percent of iron (i.e., look at the 99 % CL). In this case, the calculated range **does** encompass the theoretical percentage of iron. (you should do the calculations to convince yourself). At the 99% confidence limit you cannot be sure that the experimentally determined percentage of iron is actually lower than the theoretically predicted amount. Thus you can say you are between 90-99 % confident that your compound contains less iron than that expected.

In this case, you should then attempt to explain why your experimentally determined value may be lower than the theoretical predicted amount (think about what you measured in the experiment and where errors could have been introduced[1]).

You should also do this type of analysis for the oxalate analysis. Remember use your data.

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[1] Human error is not an acceptable explanation – citing human error basically tells the reader that you did not do the work carefully and could call into question the reliability of all of your data. The point of this