

## Calculating cmc and Q/N

1. Transcribe your concentration and conductivity results into columns A and B of an Excel spreadsheet. Prepare a graph of conductivity (y-axis) versus surfactant concentration (x-axis). From looking at your graph, *estimate* the concentration at which two straight lines would intersect: this should correspond to the critical micelle concentration, or *cmc*.
2. Your data should look like two straight line segments. To find the intersection between these two lines, you need to fit the data by linear regression. Trendline is the quickest way to do this, but is not the best way if you need to know uncertainty. First, fit each of the two segments using Trendline, and decide which points belong to which line. Show both equations and  $R^2$  values for now, and note them down, but don't include them on any Figures in your final presentation.
3. A more complete way of doing the analysis is to use The **Data Analysis** package on the **Data** tab. Double-click to open a pop-up, and choose **Regression**. This will allow you to highlight your x and y data ranges for your first line segment fit, and also an **Output Range** for the results. Choose a single cell on the current worksheet somewhere away from your data and graph. You don't need to make a new plot. This will give you a summary output that looks something like this:

SUMMARY OUTPUT								
<b>Regression Statistics</b>								
Multiple R	0.999638							
R Square	0.999275							
Adjusted R	0.99913							
Standard E	0.06351							
Observations	7							
<b>ANOVA</b>								
	<i>df</i>	<i>SS</i>	<i>MS</i>	<i>F</i>	<i>Significance F</i>			
Regression	1	27.81232	27.81232	6895.208	4.8E-09			
Residual	5	0.020168	0.004034					
Total	6	27.83248						
<b>Coefficients</b>								
	<i>Coefficients</i>	<i>Standard Error</i>	<i>t Stat</i>	<i>P-value</i>	<i>Lower 95%</i>	<i>Upper 95%</i>	<i>Lower 95.0%</i>	<i>Upper 95.0%</i>
Intercept	0.011786	0.043275	0.272344	0.796246	-0.09946	0.123028	-0.09946	0.123028
X Variable	0.996643	0.012002	83.03739	4.8E-09	0.96579	1.027496	0.96579	1.027496

The main things to notice are the **Intercept** and **X Variable** (slope), which should be the same as your Trendline equation. Notice that this output also gives  $R^2$  (called **R Square**). More importantly, it gives you the **Standard Error** in your slope and intercept in the column next to the values themselves. Further across you can see the Lower 95% and Upper 95% confidence limits, which correspond to the best fit value of each quantity  $\pm 2 \times \text{Standard Error}$ , which we use as the uncertainty or error.

Do this for both line segments of your conductivity results.

4. The intersection of two straight lines given by  $y_1 = m_1x + b_1$  (above the cmc) and  $y_2 = m_2x + b_2$  (below the cmc), is easily calculated by finding  $y_1 = y_2$ , or  $y_1 - y_2 = 0$ . This gives  $x_0 = \text{cmc} = \frac{b_2 - b_1}{m_1 - m_2}$ . Calculate this best-fit value of the intersection,  $x_0$ , for your data, and equals the *cmc*. Is it near your estimated value from step 2?

5. You can also use the ratio of your best fit slopes  $m_1$  and  $m_2$  to calculate  $1-Q/N$ , and hence  $Q/N$ .

Now we come to the uncertainty, which will tell you how many figures are significant. Here we will assume that the uncertainties in the concentrations of surfactants from dispensing and volumetric glassware are negligible, and focus on the error in fitting conductivity data

6. You can calculate this by unpacking the equation for the intersection. As it is a quotient (see Expt 1 worksheet), we can write the error in terms of fractional errors of the numerator and denominator

$$\frac{\sigma_{cmc}}{cmc} = \left( \left( \frac{\sigma_{b_2 - b_1}}{b_2 - b_1} \right)^2 + \left( \frac{\sigma_{m_1 - m_2}}{m_1 - m_2} \right)^2 \right)^{1/2}$$

That's not very useful yet, but notice that the *fractional error* depends on the difference between the slopes and intercepts of the two lines. This should make sense: It should be easier to accurately find the intersection between two lines with very different slopes or intercepts than two lines that nearly lie on top of each other.

The error in  $b_2 - b_1$  or in  $m_1 - m_2$  can be calculated from the errors in the individual slopes and intercepts. This gives us a messy but straightforward equation overall:

$$\frac{\sigma_{cmc}}{cmc} = \left( \left( \frac{\sigma_{b_2}}{b_2 - b_1} \right)^2 + \left( \frac{\sigma_{b_1}}{b_2 - b_1} \right)^2 + \left( \frac{\sigma_{m_1}}{m_1 - m_2} \right)^2 + \left( \frac{\sigma_{m_2}}{m_1 - m_2} \right)^2 \right)^{1/2}$$

Use this to calculate the uncertainty in your intersection.

You should now be able to write your intersection value with error to the correct number of significant figures.

**Remember, the uncertainty is expressed to one or two digits (between 03 and 30 - see Appendix 2) and the quantity itself is rounded off to be consistent with the number of decimal places in the uncertainty.**

7. The error in  $Q/N$  is much simpler to calculate.  $Q/N = 1 - m_1/m_2$ . As there is no uncertainty in '1', the error in  $Q/N$  is the same as the error in  $m_1/m_2$  or

$$\frac{\sigma_{Q/N}}{Q/N} = \left( \left( \frac{\sigma_{m_1}}{m_1} \right)^2 + \left( \frac{\sigma_{m_2}}{m_2} \right)^2 \right)^{1/2}$$

You should now also be able to write the value of  $Q/N$  with error to the correct number of significant figures.

8. Finally, you can calculate  $\Delta G^\circ_{mic} = (1 + Q/N)RT \ln(cmc)$ , with uncertainty, of course. Remember that the  $cmc$  must be expressed M for this calculation, as the standard state for aqueous solutions is 1 M.

9. As  $\Delta G^\circ_{mic}$  involves the product of two experimental quantities,  $cmc$  and  $Q/N$ , the uncertainties in both must be accounted for.

First, consider the uncertainty in  $\ln(cmc)$ . We can use function error analysis (see Appendix 2), but for a one-off calculation, try thinking about errors as representing a range for the correct answer. That is, if we measure the  $cmc$  again, we'd expect it to fall between  $(cmc - \sigma_{cmc})$  and  $(cmc + \sigma_{cmc})$  95% of the time.

You can take the same approach to  $\ln(cmc)$ : 95% of repeat measurements will fall between  $\ln(cmc - \sigma_{cmc})$  and  $\ln(cmc + \sigma_{cmc})$ . If you calculate these two values, you should see that the *fractional error* in  $\ln(cmc)$  is much smaller than that in  $cmc$ . This is a general property of logarithms. **This means that the uncertainty in  $\Delta G^\circ_{mic}$  is mostly determined by the uncertainty in  $Q/N$ , so you can neglect the uncertainty in  $\ln(cmc)$ .** You should now be able to write down  $\Delta G^\circ_{mic}$  to the correct number of significant figures, with its uncertainty.