CHM 317H1S
Winter 2021

Statistical Tables, Significant Figures, Error Propagation, and Data Analysis

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Statistical Tables

1. Critical values for Grubb's test at the 95% CL (P = 0.05)

n	G_{crit}	n	G_{crit}	n	G_{crit}
3	1.154	7	2.020	14	2.507
4	1.481	8	2.127	20	2.708
5	1.715	9	2.215	30	2.909
6	1.887	10	2.290	50	3.128

Calculate G for the most extreme value (minimum *or* maximum) and look up the critical value G_{crit} in the table above:

$$G = \frac{|x_{suspect} - \bar{x}|}{s}$$ *May* reject $x_{suspect}$ as an outlier if $G > G_{crit}$

2. Values of the *t*-statistic at the 95% CL (P = 0.05) for a 2-tailed test

$\nu = (n-1)$	t_{crit}	$\nu = (n-1)$	t_{crit}	$\nu = (n-1)$	t_{crit}
1	12.706	6	2.447	15	2.131
2	4.303	7	2.365	20	2.086
3	3.182	8	2.306	25	2.060
4	2.776	9	2.262	30	2.04
5	2.571	10	2.228		

For a *t*-test, calculate the value of t and look up the critical value t_{crit} in the table above. For example, to compare a sample mean with a true value:

$$t = \frac{|m - \bar{x}|\sqrt{n}}{s}$$ *The sample mean is not from the parent population if* $t > t_{crit}$

To calculate a confidence interval, look up the value of t from the table for the appropriate value of n and calculate:

95% Confidence interval: $m = \bar{x} \pm \frac{ts}{\sqrt{n}}$

3. Values of the *F* statistic at the 95% CL (P = 0.05) for a 1-tailed test

F_{crit}	$\nu_1 = 2$	3	4	5	6	7	8	9	10
$\nu_2 = 2$	19.00	19.16	19.25	19.30	19.33	19.35	19.37	19.38	19.40
3	9.552	9.277	9.117	9.013	8.941	8.887	8.845	8.812	8.786
4	6.944	6.591	6.388	6.256	6.163	6.094	6.041	5.999	5.964
5	5.786	5.409	5.192	5.050	4.950	4.876	4.818	4.772	4.735
6	5.143	4.757	4.534	4.387	4.284	4.207	4.147	4.099	4.060
7	4.737	4.347	4.120	3.972	3.866	3.787	3.726	3.677	3.637
8	4.459	4.066	3.838	3.687	3.581	3.500	3.438	3.388	3.347
9	4.256	3.863	3.633	3.482	3.374	3.293	3.230	3.179	3.137
10	4.103	3.708	3.478	3.326	3.217	3.135	3.072	3.020	2.978

For an *F*-test, calculate the value of F and lookup the critical value F_{crit} in the table above. Note that the *larger* standard deviation is *always* used as the numerator:

$$F = \frac{s_1^2}{s_2^2} \text{ where } s_1 > s_2 \text{ } i.e. \text{ } F > 1$$

The standard deviations are assumed to be for samples drawn from the *same* population (*i.e.* NO significant difference) if $F \leq F_{crit}$.

Tolerances for Selected Volumetric Glassware

Item	Volume (mL)*	Absolute Uncertainty (mL)	Cost ($)‡
Transfer pipette	75.00	± 0.08	n/a
	50.00	± 0.05	215.00
	30.00	± 0.04	n/a
	25.00	± 0.03	162.00
	20.00	± 0.02	151.00
	15.00	± 0.03	142.00
	10.00	± 0.02	104.00
	5.00	± 0.01	93.00
	4.00	± 0.01	93.00
	3.00	± 0.01	93.00
	2.000	± 0.006	93.00
	1.000	± 0.006	93.00
Mohr pipette†	10.00	± 0.05	100.00
	5.00	± 0.04	86.00
	2.00	± 0.02	86.00
	1.00	± 0.02	86.00
	0.100	± 0.005	91.00
Volumetric flask	1000.0	± 0.30	61.00
	500.0	± 0.15	50.00
	250.0	± 0.12	39.00
	200.0	± 0.10	37.00
	100.00	± 0.08	32.00
	50.00	± 0.05	30.00
	25.00	± 0.03	28.00
	10.00	± 0.02	26.00
	5.00	± 0.02	25.00
	1.00	± 0.01	30.00

* Volume to deliver at the mark, at a temperature of 20 °C
† Check whether pipette is 'To Deliver' (TD) or 'To Contain'
‡ 2003 Prices – adjust for inflation!

Significant Figures, Decimal Places, and Error Propagation

In any practical science, all calculations and results should take the errors and uncertainties associated with actual measurements into account. In this context, the **error** E_x in a measured value x is defined as the *actual* difference between the true and measured values: $E_x = x_{true} - x$. While such measurement errors *always* exist, it is not always possible to determine them since the true value may not be known. In most cases the best we can do is provide an *estimate* of the error, which we term the **uncertainty**; any value x therefore always has an associated uncertainty $\pm\Delta x$, which must be accounted for in any subsequent calculations. The uncertainty Δx may be due to known sources of error, random fluctuations inherent in instrumental operation, or the limiting resolution of a readout or display. Uncertainty may be expressed as an actual error (when known), an estimated error, a standard deviation, or confidence interval. Uncertainty also exists in any quantity derived from one or more measured values, and must be determined by a procedure known as **error propagation**.

1. Determining the uncertainty, Δx:

- Derived or measured values always have an **implied uncertainty** if none is stated, which is taken as ± 1 in the last significant figure. Uncertainties *always* have the same units as the value for which they provide an error estimate. For example:

$$M_m = 242.13 \pm 0.01 \text{ g/mol} \qquad E = -163 \pm 1 \text{ mV}$$
$$A = 0.137 \pm 0.001 \text{ AU} \quad C = 1.00 \times 10^{-3} \pm 1 \times 10^{-5} \text{ mol/L}$$

- When the arithmetic mean of a set of n repeated values is calculated, the uncertainty is based on the unbiased standard deviation, s. This is denoted on most calculators as either σ_{n-1} or s_{n-1} and is calculated as:

$$s = \sqrt{\frac{\sum_1^n (x_i - \bar{x})^2}{n - 1}}$$

☞ Save time and avoid simple mistakes – use your calculator for this!

Note that a standard deviation, being an estimate of the error in the mean value, only has *one* significant figure; it is customary to report the first non-significant digit also, in order to avoid premature rounding in subsequent calculations. For example:

Example 1: m = 10.0120, 10.0051, 10.0073, 10.0046, 10.0111 g

$\overline{m} = 10.008_{02}$ g, $s = 0.003_4$ g, $n = 5$

$$\therefore\ \overline{m} = \mathbf{10.008 \pm 0.003\ g\ (\overline{m} \pm s,\ n = 5)}$$

Note that, in this example, the mean value actually has *fewer* significant figures than the individual readings as a direct consequence of the value of the standard deviation!

Sometimes, an instrument is incapable of resolving the inherent variation between repeated measurements, resulting in a string of identical values with $s = 0$. In this case, the uncertainty is expressed as ±1 in the last figure of the instrument display.

Example 2: E = 107, 107, 107 mV

$$\overline{E} = 107 \text{ mV}, s = 0 \text{ mV}, n = 3$$
$$\therefore \overline{E} = 107 \pm 1 \text{ mV } (n = 3)$$

2. Error propagation with implicit uncertainties:

When performing calculations using values that have an implied uncertainty, it is essential to observe the correct rules for determining the uncertainty Δq in the final value, q, as this will determine the correct number of significant figures to which the result may be quoted.

- When adding or subtracting, the least significant digit in the result is determined by the value with the fewest decimal places.
- When multiplying or dividing, the least significant digit in the result is determined by the value with the fewest significant figures.
- When a calculation involves both types of operation (additive and multiplicative), observe the order of mathematical precedence and determine the correct numbers of significant figures for intermediate values.
- It is always advisable to retain at least the first non-significant digit in intermediate values in order to prevent premature rounding of the final result. Non-significant digits should be clearly denoted using either subscripting, underlining, or enclosing them in parentheses.

Example 3: calculate the molar mass of calcium carbonate

- $1 \times 40.08 = 40.08$
- $1 \times 12.011 = 12.011$
- $3 \times 15.9994 = 47.9982$
- $= 100.08_{92}$ $\therefore M_m(CaCO_3) = 100.09$ g/mol

- Notice how, in this example, the molar mass *correctly* has 5 significant figures, even though the atomic mass of calcium was only known to four significant figures! This is because the *largest* uncertainty in any of the masses is ±0.01 g/mol, so the error in the sum total lies in the second decimal place.

Example 4: calculate the mass of calcium carbonate required to make 100.0 mL of an 0.200 M solution:

$$C = \frac{m \text{ (g)}}{M_m \text{ (g/mol)} \times V \text{ (L)}} \therefore m = C \times M_m \times V$$

$$\therefore m = 0.200 \frac{\text{mol}}{\text{L}} \times \frac{100.0 \text{ mL}}{1000 \text{ mL/L}} \times 100.08_{92} \frac{\text{g}}{\text{mol}}$$

$$\therefore m = 2.00_{18} \text{ g} = 2.00 \text{ g of calcium carbonate}$$

Notice how, in this example, the final result can only be given to 3 significant figures, even though the volume and molar mass are known to 4 and 5 significant figures, respectively. (Remember that leading zeroes before the decimal place are *not*

counted towards the number of significant figures; we could clarify this by writing $C = 2.00 \times 10^{-1}$ M.)

When calculating logs and antilogs, remember that the number of significant figures associated with a value x determine the number of decimal places reported for log x. Similarly, the number of decimal places for a value y determines the number of significant figures reported for 10^y.

3. Error propagation with calculated uncertainties:

In analytical and physical chemistry, it is important to explicitly calculate the effect of individual uncertainties on the overall uncertainty in the final result. In fact, the rules in the preceding section are based on the mathematical procedures one must use to do this. It is therefore important to evaluate the uncertainties in additive and multiplicative steps independently, as different rules apply.

- When adding or subtracting values with random errors, *e.g.* if $q = x + y$ or $q = x - y$ then the uncertainty Δq in q is:

$$\Delta q = \pm\sqrt{(\Delta x)^2 + (\Delta y)^2}$$

Example 5: the uncertainty in the difference between two weights, each measured to the nearest ±0.0001 g:

$$m = m_{\text{final}} - m_{\text{initial}} = 23.2476 - 21.1942 \text{ g} = 2.0534 \text{ g}$$

$$\Delta m = \sqrt{(0.0001)^2 + (0.0001)^2} = \pm 0.00014 \text{ g}$$

- When multiplying or dividing values with random errors, e.g. if $q = ax \times y$ where a is a constant, the uncertainty Δq in q is:

$$\Delta q = \pm q\sqrt{\left(\frac{\Delta x}{x}\right)^2 + \left(\frac{\Delta y}{y}\right)^2}$$

Example 6: the uncertainty in the concentration obtained by dissolving 2.0534 g of $CaCO_3$ in water and making to volume in a 100.0 mL volumetric flask

- The uncertainty in the mass from above is ± 0.00014 g
- The molar mass from above is 100.09 ± 0.01 g/mol
- The uncertainty in flask volume is ± 0.08 mL

$$C = \frac{m}{M_m \times V} = \frac{2.0543 \text{ g}}{100.08_{92} \text{ g/moL}} \times \frac{1000 \text{ mL/L}}{100.0 \text{ mL}} = 2.051_{57} \times 10^{-1} \text{ mol/L}$$

$$\Delta C = \pm C\sqrt{\left(\frac{\Delta m}{m}\right)^2 + \left(\frac{\Delta V}{V}\right)^2 + \left(\frac{\Delta M_m}{M_m}\right)^2}$$

$$\therefore \Delta C = \pm 0.2051_{57}\sqrt{\left(\frac{0.0001_4}{2.0534}\right)^2 + \left(\frac{0.08}{100.0}\right)^2 + \left(\frac{0.01}{100.08_{92}}\right)^2}$$

$$\therefore \Delta C = \pm 1.66 \times 10^{-4} \text{ M} \therefore C(CaCO_3) = 0.2051_6 \pm 0.00017 \text{ mol/L}$$

4. Rounding values from calculations:

Whether dealing with implied or actual uncertainties, it is essential to round the final value correctly. Most textbooks describe the procedure adopted in computer science, and commonly

implemented on calculators, where values are rounded up if the first non-significant digit is greater than or equal to 5, but rounded down if less than 5. Unfortunately, this leads to some bias in the results for cases where the non-significant portion of the number is exactly 5. In analytical chemistry, we therefore implement a third rule: if the non-significant portion of the number is exactly 5, the result is rounded to the *nearest even number.* This means that half the time the result will be rounded *up*, and half the time it will be rounded *down*.

» In computer programming, this is sometimes referred to as "banker's rounding"; if the bank always rounded the interest on your loan up, you would be overcharged!

Example 7:

$q = 13.379_{512}$ – the non-significant digits are $> 0.000_5$ so we round **up**

$q = 227.63_{439}$ – the non-significant digits are $< 0.00_5$ so we round **down**

$q = 1.141_5$ – the non-significant digits are $= 0.000_5$; round to 1.142

$q = 10.76_5$ – the non-significant digits are $= 0.00_5$; round to 10.76

5. Outliers, Confidence Intervals, and Significance Tests:

- If you suspect that one or more values in a set of replicate measurements is an outlier, apply Grubb's test to the data to see if the suspect value can be rejected (see lab manual or the course text)
- When a final result is the average of several individual determinations, calculate the 95% confidence interval about the mean using the *t*-statistic (see lab manual or course text)
- If an experiment calls for either a comparison of the measured mean with a known true value (test of accuracy and bias) or the comparison of the standard deviations of two sets of results (test of precision), use the appropriate statistical test (*t*-test or *F*-test, respectively)

Calibration, Regression, Interpolation, and Bracketing

Most instrumental techniques require proper calibration of the instrument for accurate quantitative analysis. This is covered in detail in the course text. In addition, the course web site contains links to a self-guided tutorial on the use of Microsoft® Excel™ to perform linear regression analysis, and the correct calculation of the estimated errors in values derived from such calibration curves by either interpolation or extrapolation. This section provides a brief overview of the key points.

- Concentration is always the independent (x-axis) variable
- The number of significant figures for each axis scale is determined by the uncertainty in your standard concentrations and measured readings
- Always include a title, axis labels (with correct units), and a legend. The title should refer to the *experiment*, not simply "A plot of *y* versus *x*". So, you might have a graph titled, "Calibration Curve for the Determination of Cobalt by Absorbance at 515 nm"
- Perform your own regression analysis on your calibration data, even if the instrument or software does this for you
- *Never* force a regression line through zero (the origin); you should, however, include the blank reading if available.
- *Always* calculate the slope, intercept, standard error of the regression, and the correlation coefficient (r or r^2) for a calibration curve. You should also calculate the limit-of-detection from the regression data.
- For replicate measurements, *either* plot them as discrete values for each concentration *or* as mean values with *y*-error bars to indicate ±1 standard deviation for each standard. Clearly indicate if you have done the latter but the error bars are too small to be visible on the plot.

Note that the use of Excel™ to perform many of the above is described in the on-line tutorial on calibration and regression, complete with numerous examples and sample files that you may download. If you are unfamiliar with Excel, or any of the available statistics programs such as MAPLE, MiniTab, *etc*., you should spend some time working through this material; you will waste a lot of time writing up lab reports if you do all the calculations by hand! See:

http://sites.chem.utoronto.ca/chemistry/coursenotes/analsci/stats/

The figure on the next page summarizes the key points of calibration, regression, and the limit of detection. In order to fit a linear calibration function $y = bx + a$ to the experimental data, we use regression analysis (the mean values here are the mean *x* and *y* values for the calibration data):

Calculate the slope: $$b = \frac{\sum_i \{(x_i - \bar{x})(y_i - \bar{y})\}}{\sum_i (x_i - \bar{x})^2}$$

Calculate the intercept: $a = \bar{y} - b\bar{x}$

Calculate the correlation coefficient:

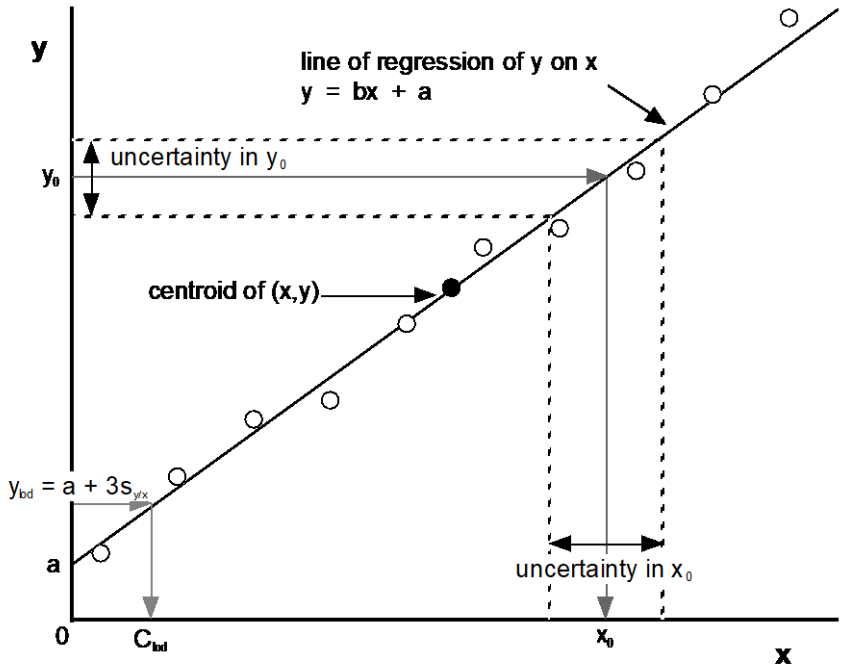
$$r = \frac{\sum_i \{(x_i - \bar{x})(y_i - \bar{y})\}}{\left[\left(\sum_i (x_i - \bar{x})^2\right)\left(\sum_i (y_i - \bar{y})^2\right)\right]^{1/2}}$$

Calculate the standard error of regression: $s_{y/x} = \sqrt{\frac{\sum_i (y_i - \hat{y}_i)^2}{n - 2}}$

Note that many of these values can be calculated in Excel easily using the built-in LINEST function. For details, please see the on-line stats tutorial page on errors in regression analysis (http://www.chem.utoronto.ca/coursenotes/analsci/stats/ErrRegr.html).

1. Limit-of-Detection and Quantitation:

For linear response–concentration calibration plots, you should always calculate the limit-of-detection for your method and measurement conditions. In chemical measurement, this is defined as *the concentration giving the smallest detectable signal above the baseline (background) noise*. Technically, this should be calculated based on repeat measurement of a blank (sample matrix with *no* analyte present). Practically, this is often unfeasible due to time constraints. A common alternative is to use the calibration data and regression line, as shown:



Line of regression of y (instrument response) on x (concentration) using least–squares, showing the concentration limit-of-detection (lod) and the determination of an unknown concentration x_0 from a measured response y_0

To calculate the limit-of-detection:

1. Determine the smallest detectable signal, y_{lod}, as *either*:

– the blank plus three times the standard deviation of the blank ($n > 20$)

$$y_{\text{lod}} = y_{\text{blank}} + 3s_{\text{blank}}$$

– the intercept, a, plus three times the standard error of the regression

$$y_{\text{lod}} = a + 3s_{y/x}$$

2. Convert the value of y_{lod} into the corresponding concentration limit-of-detection using the calibration equation from the regression analysis:

$$C_{lod} = \frac{y_{lod} - a}{b}$$

Note that, when using the regression line, steps 1 and 2 can be combined to yield a simplified form of the equation:

$$C_{lod} = \frac{3s_{y/x}}{b}$$

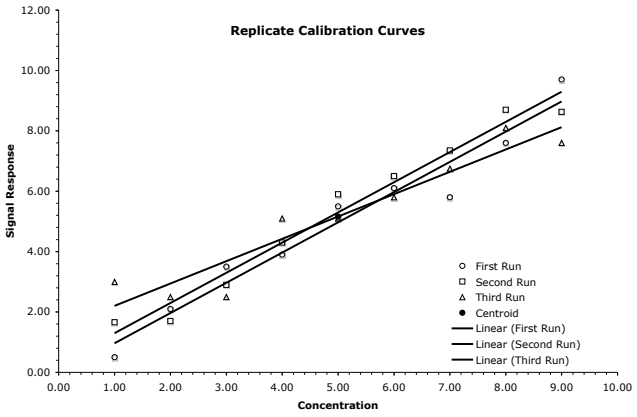
Similarly, we can calculate the lowest concentration that can be determined by interpolation through the calibration graph, known as the ***limit of quantitation***. This is determined using the same formula as the limit of detection, with the exception that we use a factor of 10 instead of 3 in the formula.

2. Interpolating a Value:

In order to calculate the concentration of a sample from its measured response, you will need to make an interpolation of the response, y_0, using the response equation derived from your regression analysis. The uncertainty in the resulting concentration, x_0, can be calculated from the regression statistics as demonstrated in the on-line tutorial and lecture material. Note that the *smallest* error is obtained when the measured response (y_0) and concentration (x_0) correspond to the centroid (mean of x and y) of the data; the further the point from the centroid, the greater the error. This is illustrated in the graph below, which shows the results of three separate sets of calibration measurements obtained using the same standards, instrument, and method (the errors in each measurement have been exaggerated for the purpose of illustration.)

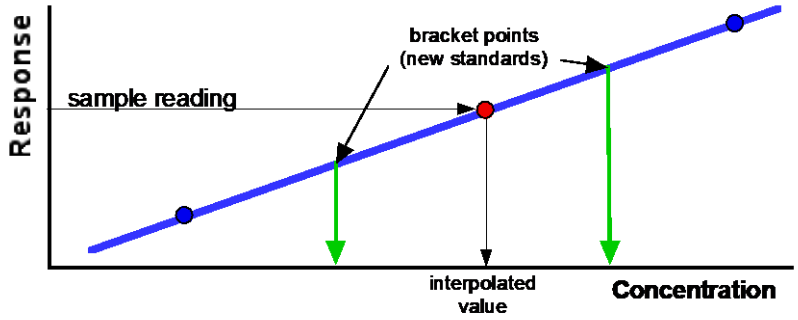
For an interpolated value, the standard error in that value is (m is the number of measurements for the sample value y_0, n is the number of points in the calibration data, and other symbols are as defined above:

$$s_{x_0} = \frac{s_{y/x}}{b}\sqrt{\frac{1}{m} + \frac{1}{n} + \frac{(y_0 - \bar{y})^2}{b^2 \sum_i (x_i - \bar{x})^2}}$$



3. Bracketing the sample concentration:

One consequence of the increased uncertainty in interpolated values away from the centroid of the calibration data is that, in order to get meaningful results, it is often necessary to *bracket* your sample data points. This means that you obtain additional calibration points on either side of your experimental data, and perform regression analysis on this smaller sub-set of your calibration data. This is illustrated graphically below:



Bracketing a sample point by adding new standards to the calibration curve

Once you have identified target concentrations for additional standards, you can calculate the dilution factor required to obtain that value from one or more of your existing stock or standard solutions. You can then find the combination of transfer pipette and volumetric flask that most closely yield these values *without* using up large amounts of standard and solvent. For example, consider the following scenario:

Stock concentration, $C_{stock} = 0.1005$ M
Standards: $C_1 = 0.001005$ M, $C_2 = 0.002010$ M, $C_3 = 0.005025$ M, $C_4 = 0.01005$ M
Initial sample estimate: $C = 0.00132$ M

Since the sample is at the extreme end of the calibration range, we would want at least one extra standard midway between the first two at ~ 0.001507 M:

Dilution factor required using stock solution, $f = \dfrac{0.001507}{0.1005} = 0.01499 \approx 0.015$

To get this, we could use a 15.00 mL pipette and a 1.000 L flask, but this would generate a lot of waste! We could also dilute 15.00 mL of the fourth standard (0.01005 M) to 100.0 mL, which is more reasonable:

$$C_{dilute} = C_4 \times \frac{V_{pipette}}{V_{flask}} = 0.01005 \times \frac{15.00}{100.0} = 0.001507_5 \text{ M}$$

4. Extrapolating a Value:

Normally in analytical chemistry we avoid extrapolating calibration curves for the simple reason that the uncertainties arising from the regression line are greatest at the extreme ends of the calibration range. The *relative error* will also be greatest where you have both large uncertainties and small values. Sometimes, however, specific techniques require the use of extrapolation in order to determine a value. One example of this is the method of standard additions. In its simplest form, this requires extrapolating a linear equation to the intercept on the x-axis, x_E, as shown on the next page.

The method works by first assuming that any interfering species in the sample will affect the signal due to the analyte by the same relative amount *regardless* of the analyte concentration. Suppose, for example, that the calibration curve for the analyte in the *absence* of any interferent was:

$$I = bC$$

If an interferent reduces the measured signal I by a fixed fraction f, then the calibration curve in the *presence* of the interferent will be:

$$I¢= fbC$$

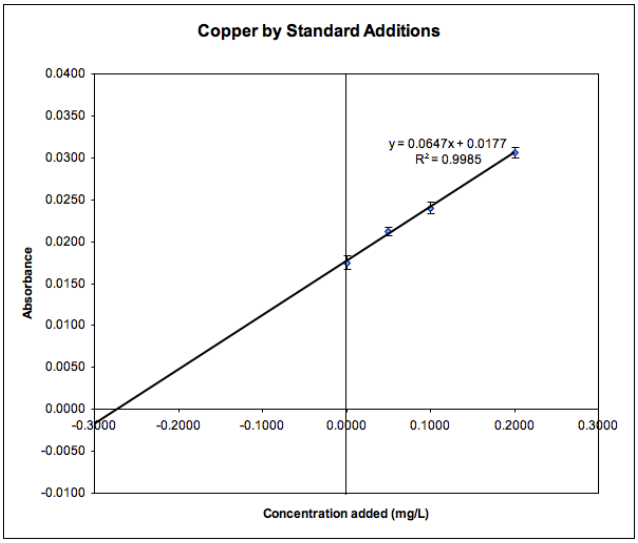
Note that when $C = 0$, $I = I' = 0$. In standard additions, increasing amounts of a standard (C_s, V_s) are added to a fixed amount of sample (C_o, V_o). Assuming that each portion of sample with added standard is diluted to the same total volume (V_T) then we can derive the equation:

$$I' = fbC = fb\left(\frac{C_o V_o}{V_T} + \frac{C_s V_s}{V_T}\right) = fbC_x + fbC_{add}$$

From this, we can see that a plot of I' versus C_{add} will have an intercept on the x axis ($I' = 0$) equal to $-C_x$. The uncertainty, or standard error, of the intercept obtained in this manner can be calculated from the regression statistics as:

$$s_{x_E} = \frac{s_{y/x}}{b}\sqrt{\frac{1}{n} + \frac{\bar{y}^2}{b^2 å\left(x_i - \bar{x}\right)^2}}$$

Once again, n is the number of points in the calibration curve, b is the slope, and the means refer to the mean x and y values for the calibration data.



Standard additions plot for the determination of copper by flame AAS

Functional Group Correlation Tables for FTIR

The following tables provide ***approximate ranges*** for the IR absorption bands of common organic functional groups and structural elements. Please note that the precise location of a band depends on the specific compound being studied. For example, the intense carbonyl stretching frequency can vary slightly between different ketones.

- **Bond X–Y (Z)**: the term in brackets denotes whether the absorption band is for a **s**tretch or **d**eformation; oop = out-of-plane, ip = in plane
- The relative magnitude of absorption or decrease in %T is indicated following the wavenumber range as: **s** – strong; **m** – medium; **w** – weak; **v** – variable

Group	Bond	ν / cm^{-1}		Remark
Alkane	C–H (S)	2975–2950	m	asym. CH_3
		2885–2860	m	sym. CH_3
		2940–2915	m	asym. CH_2
		2870–2845	m	sym. CH_2
		2900–2880	w	tertiary CH
	C–CH_3 (D)	1470–1430	m	asym.
		1380–1370	s	sym.
	–CH_2– (D)	1485–1445	m	
	–CH–	≈1340	w	
Alkene	C=C (S)	1680–1620	v	non-conjugated
		≈1625	v	Phenyl-conjugated
		≈1600	v	C=O or C=C conj.
	–CH=CH– (trans)	3040–3010	m	trans CH (S)
		970–960	s	trans CH (oop D)
		1310–1295	v	trans CH (ip D)
	–CH=CH– (cis)	3040–3010	m	cis CH (S)
		≈690		cis CH (oop D)
	–$CH=CH_2$	3095–3075	m	CH (S)
		995–985	s	CH (oop D)
		915–905	s	CH_2 (oop D)
		1850–1800	m	CH_2 overtone
		1420–1410	s	CH_2 (ip D)
		1300–1290	v	CH (ip D)
Aromatic	C–H (S)	3080–3030	m	several bands
		2000–1660	v	
	C=C (S)	≈1600	v	skeletal vibrations
		≈1500	v	skeletal vibrations
		≈1580	m	skeletal (conjugated rings)
		≈1450	m	skeletal (conjugated rings)
	C–H (D)	770–730	s	monosubstituted
		710–690		monosubstituted
		770–735	s	ortho disubstituted
		900–860	s	meta disubstituted
		810–750	s	meta disubstituted
		860–800	s	para disubstituted
Alkyl halide	C–F (S)	1400-1000	s	
	C-Cl (S)	600-800	s	
	C-Br (S)	500-600	s	
	C-I (S)	500	s	

Group	Bond	ν / cm^{-1}		Remark
Alcohol	O–H (S)	3670–3580	s	free O–H
	O–H (S)	3400–3230	s	H-bonded O–H
	C–O (S)	1075–1000	s	primary aliphatic
	C–O (S)	1230–1140	s	aromatic
Ether	C–O (S)	1175–1050	s	Aliphatic CH_2–O–CH_2
		625-500	m	
		1300–1175	s	Aromatic Ar–O–CH_2
		1070–1000	m	
Aldehyde	C=O (S)	1715–1695	s	aromatic
	C=O (S)	1740–1720	s	sat. aliphatic
	C–H (S)	2880–2650	w	can be 2 bands
Ketone C=O	R–CO–R	1725–1700	s	C=O (S)
	R'–CO–R	1685–1660		C=C–C=O conj.
	R–CO–Ar	1700–1680		alkyl–aryl C=O (S)
	Ar–CO–Ar	1670–1660		aryl C=O (S)
	diketone	1730–1710		
	enolized	1640–1540		R–CO–CH2–CO–R
	sat. cyclic	1725–1705		6+ ring
		1750–1740		C=O on 5 member ring
		1775		C=O on 4 member ring
	quinone	1690–1660		C=O on same ring
		1655–1635		C=O on diff. ring
Acid C=O	R–COOH	1725–1700		acid dimer (H-bonded)
		1715–1650		C=C conj., dimer
	Ar–COOH	1700–1680		Aromatic acid
Ester	C=O (S)	1750–1735	s	
	C–O (S)	1250–1230	s	acetates
	C–O (S)	1200–1180	s	formates, others
Anhydride	C=O (S)	1850–1700	s	Linear C–CO–O–CO–C (2 bands)
		1875–1725	s	Cyclic –CO–O–CO– (2 bands)
Amine	N–H (S)	3500–3300	m	Free N–H; 2 bands in primary
		3400-3100	m	H-bonded N–H
	C–N (S)	1360–1250	m	Aryl amines
		1200-1000	m	Alkyl amines
	N–H (D)	1650–1550	m	In-plane bend
		800-700	m	o.o.p. bend
Amide	N–H (S)	3360–3180	s	2 bands in primary (broad)
	C=O (S)	1740–1650	s	All amides
		1650–1550	m	Primary amide
		1600-1480	m	Mono-substituted amide
Nitrile	–C≡N (S)	~2250	s	Aliphatic
		~2230	s	Aromatic
Isocyanide	–N≡C (S)	2100-2000		
Isocyanate	N=C=O (S)	2400–2100		C= N & C=O (broad)
Nitro	N–O (S)	1550-1475	s	Asymmetric stretch
		1360-1290	s	Symmetric stretch
Silicones	Si–CH_3 (D)	1270 cm^{-1}		Symmetrical deformation
Siloxanes	Si–O–Si (S)	1100, 1040 cm^{-1}		
Sulphonates	–O–SO_3^- (D)	620–560		Deformation
	–O–SO_3^- (S)	1230–1180		Asymmetric stretch
		1080–1020		Symmetric stretch