

you-try-it-03.xlsx
Step-by-Step Guide
ver. 8/5/2016

Abstract

This document provides step-by-step instructions for the Excel workbook you-try-it-03.xlsx (saved from Excel 2010). The worksheets contain data for practice exercises keyed to Chapter 3 of:

Basics of Analytical Chemistry and Chemical Equilibria by Brian M. Tissue
(John Wiley: New York, 2013).

<u>Worksheets in the workbook</u>	<u>page in this guide</u>
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General Advice

It is often useful to work out or outline the first example on each worksheet on paper. After obtaining a result, compare your result to the answer in this guide. Next write formulas on the worksheet to do the calculations. If your formulas do not produce the same answer, try writing them step-by-step and compare intermediate results to calculations on paper to find errors. Try to write formulas to be general so that you can copy them to use for multiple cases.

Version History

9/2/2009	First posting.
8/5/2016	Formatting revisions.

For updates visit the text support website:

<http://www.achem.org>

3.A limiting-reagent

This worksheet contains a table of different types of reactions. Often when adapting a procedure for a larger than normal amount of sample, the amount of reagents must be checked so that they do not affect the accuracy of the analysis. For each reaction we wish to determine the minimum amount of reagent that is needed to completely react with the analyte. Knowing this information, we can then add an excess amount of reagent to ensure complete reaction of the analyte to product. Before attempting a calculation, be sure that you have a balanced reaction.

Concepts	Concept Synopsis
stoichiometry	Molecules form and reactions occur with a fixed ratio between the atomic constituents.
limiting reagent	A limiting reagent is a reactant that is consumed completely in a reaction. In sample processing and analytical reactions, we usually add reagents in excess to ensure quantitative conversion of the analyte.

1. Determine the minimum concentration of HCl to neutralize the CaCO₃.

	A	B	C	D	E	F	G	H
14		Table 3.A.1						
15		analyte	reagents	products	reaction type, sample, and procedure			
16		CaCO ₃	H ⁺	CO ₂ (g)	neutralization			
17			(x M HCl)	Ca ²⁺ (aq)	CaCO ₃ in soil (assume 5 % CaCO ₃)			
18					dry soil sample and grind to fine powder			
19					add 25 mL of HCl solution to beaker and weigh			
20					add 3.0 g of soil to beaker, swirl, reweigh after 30 min			
21					CaCO ₃ is determined from the weight loss using:			
22					CaCO ₃ (s) + 2H ⁺ (aq) → Ca ²⁺ (aq) + CO ₂ (g) + H ₂ O			

Note in the reaction that there are 2 moles of acid needed per 1 mole of calcium carbonate.

First, outline the calculation:

- convert g of soil to mol of CaCO₃:
(g soil) → (g CaCO₃) → (mol CaCO₃)
- convert mol of CaCO₃ to mol of HCl using the reaction stoichiometry:
(mol CaCO₃) → (mol HCl)
- determine concentration of HCl from mol of HCl and the volume:
(mol HCl) → (mol/L HCl)

To translate this outline to Excel, I retype the reaction data into cells that I can reference. A table with labels like the following will work. By including the units below the values I can check the dimensions of each step.

	A	B	C	D	E
24		mass soil	frac CaCO ₃	f.w. CaCO ₃	rexn stoich
25		3	0.05	100.09	2
26		g soil	g CaCO ₃ / g soil	g/mol	mol H ⁺ /CaCO ₃

In cell F24 I type the label 'moles HCl' and in cell F25 I type the formula:

$$=B25*C25*E25/D25$$

This formula calculates both steps 1 and 2 from the outline above. For step 3 of the outline, I enter the solution volume of 0.025 L (25 mL) in cell G25 and in cell H25 I type the formula:

$$=F25/G25$$

Adding labels and formatting produces something like the following figure. I highlight each calculation and I copy the formulas below the result.

	A	B	C	D	E	F	G	H
23								
24		mass soil	frac CaCO ₃	f.w. CaCO ₃	rexn stoich	moles HCl	soln vol	conc HCl
25		3.0	0.05	100.09	2	0.00300	0.025	0.12
26		g soil	g CaCO ₃ / g soil	g/mol	mol H ⁺ /CaCO ₃	mol	L	M
27						=B25*C25*E25/D25		=F25/G25

This result gives me the lowest concentration that I need to neutralize the CaCO₃ (assuming 5 % CaCO₃) in the soil. In practice, this type of analysis is done with HCl solutions of 1 – 3 M.

2. Determine the minimum volume of 0.5 M NaCl for complete reaction to AgCl₄³⁻.

The calculation is similar to the first reaction, but the details are different. I set up a table of data in rows 37-39:

	A	B	C	D	E	F	G	H
30		Table 3.A.2						
31		analyte	reagents	products	reaction type, sample, and procedure			
32		Ag ⁺	Cl ⁻	AgCl ₄ ³⁻ (aq)	complexation			
33			(0.5 M NaCl)		50.0 mL of 0.001 M AgNO ₃			
34					Ag ⁺ precipitates as AgCl in the presence of Cl ⁻			
35					an excess of Cl ⁻ can redissolve the Ag ⁺ as Ag-Cl complexes			
36								
37		vol AgNO ₃	conc AgNO ₃	moles Ag ⁺	rexn stoich			
38		0.050	0.001		4			
39		L	mol/L	mol	mol Cl ⁻ /mol Ag ⁺			

From the reaction product I know that there are 4 moles of chloride ion per 1 mole of silver ion. Outlining

the calculation:

1. convert volume and concentration of AgNO₃ solution to moles of Ag⁺:

$$(\text{vol AgNO}_3)(\text{conc AgNO}_3)(1 \text{ mol Ag}^+ / 1 \text{ mol AgNO}_3) \rightarrow (\text{mol Ag}^+)$$

2. convert mol of Ag⁺ to mol of Cl⁻ using the reaction stoichiometry:

$$(\text{mol Ag}^+)(4 \text{ mol Cl}^- / 1 \text{ mol Ag}^+) \rightarrow (\text{mol Cl}^-)$$

3. determine volume of NaCl solution from mol of Cl⁻ and the NaCl concentration:

$$(\text{mol Cl}^-) / (\text{mol/L NaCl}) \rightarrow (\text{vol NaCl})$$

In cell D38 I type the formula:

$$=B38*C38$$

In cell F37 I type the label 'moles Cl⁻' and in cell F38 I type the formula:

$$=D38*E38$$

I now have mol Cl⁻ to use for step 3 of the outline above. I enter the NaCl solution concentration of 0.5 M in cell G38 and in cell H38 I type the formula:

$$=1000*F38/G38$$

The factor of 1000 in this formula is (1000 mL)/(1 L) to convert L to mL. The final result, with labels and highlighting will look like:

	A	B	C	D	E	F	G	H
36								
37		vol AgNO ₃	conc AgNO ₃	moles Ag ⁺	rexn stoich	moles Cl ⁻	NaCl conc	NaCl vol
38		0.050	0.001	0.00005	4	0.0002	0.500	0.400
39		L	mol/L	mol	mol Cl ⁻ /mol Ag ⁺	mol	M	mL
40				=B38*C38		=D38*E38		=1000*F38/G38

This result predicts the minimum amount of 0.5 M NaCl for complete reaction. In practice, this type of reaction involving both a precipitate and a complex is more complicated, and we'll consider such multiple equilibria in Chapter 8.

3. Determine the minimum number of moles of succinic acid for complete reaction.

This procedure uses a homogeneous precipitation to slowly generate the precipitating agent from a precursor reagent. In this case the urea, $(\text{NH}_2)_2\text{CO}$, decomposes to ammonia on heating to make the solution alkaline and generate the product, $\text{Al}(\text{succ})_2\text{OH}$ (succ is an abbreviated symbol for the succinate ligand, $\text{C}_2\text{H}_4(\text{COO})_2^{2-}$).

I set up a table of data in rows 51-53. The figure also shows the calculational results that are described below.

	A	B	C	D	E	F	G	H
43		Table 3.A.3						
44		analyte	reagents	products	reaction type, sample, and procedure			
45		Al	$\text{C}_2\text{H}_4(\text{COOH})_2$	$\text{Al}(\text{succ})_2\text{OH} (s)$	precipitation of aluminum in antacid tablets			
46			urea (OH^-)		assume 0.20 g of aluminum hydroxide in a typical sample			
47					The samples are dissolved with succinic acid and urea			
48					heating the solution produces ammonia homogeneously			
49					the slow rise in pH precipitates the product			
50								
51		mass $\text{Al}(\text{OH})_3$	f.w. $\text{Al}(\text{OH})_3$	moles $\text{Al}(\text{OH})_3$	moles Al^{3+}	rexn stoich	moles succ	
52		0.20	78.004	0.00256	0.00256	2	0.0051	
53		g	g/mol	mol	mol	mol succ/mol Al	mol	
54				=B52/C52	=D52		=D52*E52	

First I find moles of $\text{Al}(\text{OH})_3$ from the given mass and formula weight. In cell D52 I type the formula:

$$=B52*C52$$

In cell E52 I type the formula:

$$=D52$$

I often skip this step for the one-to-one ratios, but I use it here as a reminder. From the reaction product I know that there are 2 moles of succinate per 1 mole of aluminum ion in the complexation reaction. Using this stoichiometry from cell F52, in cell G52 I type the formula:

$$=D52*E52$$

Since the question asked for moles of succinate, this is the final answer.

4. Determine the minimum volume of 2 % KI solution necessary for complete reaction of the Cl₂.

In this procedure 100 L of air is bubbled through a KI solution. The Cl₂ in the air reacts with I⁻ in solution to form Cl⁻ and I₂. Measuring the I₂ concentration then allows determination of the amount of Cl₂ that was in the air sample. Starting a table of data in rows 64-66, where the 'vol conv' is a volume conversion between L and m³:

	A	B	C	D	E	F	G
56		Table 3.A.4					
57		analyte	reagents	products	reaction type, sample, and procedure		
58		Cl ₂	I ⁻	I ₂ (aq)	redox		
59			(2 % KI)	Cl ⁻ (aq)	100 L of air containing 0.1 mg/m ³ Cl ₂ .		
60					bubbling air through 2 % KI solution causes:		
61					Cl ₂ + 2KI → I ₂ + 2KCl		
62					The I ₂ product is determined by titration.		
63							
64		vol air	vol conv	conc Cl₂			
65		100	0.001	0.1			
66		L	m ³ /L	mg/m ³			

In cell E64 I type the label 'mass Cl₂' and in cell E65 I type:

$$=B65*C65*D65/1000$$

The factor of 1000 is (1000 mg)/(1 g) to convert mg to g. Dividing this result by the formula weight of Cl₂ give moles Cl₂. In cell F65 I enter the formula weight of chlorine gas, in cell G64 I type the label 'moles Cl₂' and in cell G65 I type:

$$=E65/F65$$

I enter the reaction stoichiometry of 2 mol I⁻ per 1 mol Cl₂ in cell H65 and I convert to moles of I⁻ in cell I65 by typing:

$$=G65*H65$$

The result will look something like:

	A	B	C	D	E	F	G	H	I
63									
64		vol air	vol conv	conc Cl ₂	mass Cl ₂	f.w. Cl ₂	moles Cl ₂	rexn stoich	moles KI
65		100	0.001	0.1	1.00E-05	70.906	1.41E-07	2	2.82E-07
66		L	m ³ /L	mg/m ³	g	g/mol	mol	mol I ⁻ /mol Cl ₂	mol
67					=B65*C65*D65/1000		=E65/F65		=G65*H65

To make figures for this guide, I continue my calculation in cell B70 by typing =I65. You can continue your calculation in a single row. Since the KI solution is given in weight per cent, I convert to mass of KI. I enter the formula weight of KI in cell C70 and in cell D70 I type:

$$=B70*C70$$

I enter the KI concentration of 2 % as 0.02 g KI per 1 g solution in cell E70. Dividing the mass of KI necessary for complete reaction with this concentration gives the minimum mass of solution. In cell F70 I type:

$$=D70/E70$$

Finally, I convert the mass of solution to volume using the solution density (from the CRC Handbook). In cell H70 I type:

$$=F70/G70$$

The full results are shown in the next figure:

	A	B	C	D	E	F	G	H	I
63									
64		vol air	vol conv	conc Cl ₂	mass Cl ₂	f.w. Cl ₂	moles Cl ₂	rexn stoich	moles KI
65		100	0.001	0.1	1.00E-05	70.906	1.41E-07	2	2.82E-07
66		L	m ³ /L	mg/m ³	g	g/mol	mol	mol I ⁻ /mol Cl ₂	mol
67					=B65*C65*D65/1000		=E65/F65		=G65*H65
68									
69		moles KI	f.w. KI	mass KI	KI conc	mass soln	soln density	vol soln	
70		2.82E-07	166.003	4.7E-05	0.02	2.3E-03	1.01	2.3E-03	
71		mol	g/mol	g	g KI/g soln	g	g/mL	mL	
72				=B70*C70		=D70/E70		=F70/G70	

The amount of KI solution that is needed for the reaction is quite small. The amount of solution used in the bubbler will be 5 – 50 mL to ensure that all of the Cl₂ gas is captured and reacted in solution.

5. Determine the minimum number of moles of O₂ for complete combustion.

	A	B	C	D	E	F	G
75		Table 3.A.5					
76		analyte	reagents	products	reaction type, sample, and procedure		
77		C and H	O ₂	CO ₂ (g)	elemental analysis of hydrocarbon		
78				H ₂ O (g)	100 mg of paraffin wax		
79					the wax consists of equal weights of:		
80					C ₂₈ H ₅₈ , C ₃₀ H ₆₂ , C ₃₂ H ₆₆ , and C ₃₄ H ₇₀ .		

This calculation is slightly different from the others. Since we start with a mixture, we must extract the moles of C and H from each component. I set up a table in rows 82-86 for each wax component:

	A	B	C	D
81				
82		component	mass (g)	f.w. (g/mol)
83		C ₂₈ H ₅₈	0.025	394.76
84		C ₃₀ H ₆₂	0.025	422.81
85		C ₃₂ H ₆₆	0.025	450.87
86		C ₃₄ H ₇₀	0.025	478.92

Since I know that I have a total sample of 100 mg and equal weights of each component, I enter 0.025 g for each. I find the formula weights from formula-wt-calculator.xlsx and enter them in column D. Dividing the mass of each wax component by the formula weight gives the number of moles of each component. I illustrate the calculation using C₂₈H₅₈ in row 83.

To find the mol of C and mol of H for C₂₈H₅₈, calculate the mol of the compound from the mass and formula weight and then multiply by the C and H stoichiometry, respectively. In cell E83 I enter:

$$=C83/D83$$

To be able to refer to cell locations rather than typing numbers in formulas, in cell F83 I enter 28 for the number of C atoms and in cell G83 I enter the following formula for the number of H atoms:

$$=2*F83+2$$

Now I can calculate mol of C and mol of H in cells H83 and I83, respectively, using:

$$=E83*F83 \text{ and } =E83*G83$$

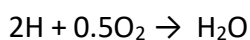
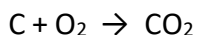
Highlight cells E83:I83 and copy downward for the whole table. Change the number of carbon atoms in column F for each case. Add labels to the table and the results will look like:

	A	B	C	D	E	F	G	H	I
82		component	mass (g)	f.w. (g/mol)	mol wax	# C	# H	mol C	mol H
83		C ₂₈ H ₅₈	0.025	394.76	6.33E-05	28	58	1.77E-03	3.67E-03
84		C ₃₀ H ₆₂	0.025	422.81	5.91E-05	30	62	1.77E-03	3.67E-03
85		C ₃₂ H ₆₆	0.025	450.87	5.54E-05	32	66	1.77E-03	3.66E-03
86		C ₃₄ H ₇₀	0.025	478.92	5.22E-05	34	70	1.77E-03	3.65E-03

The amount of oxygen required for the combustion analysis will be the amount needed to convert all of the carbon to CO₂ and all of the hydrogen to H₂O. The total amount of carbon is the sum of the results in column H and the total amount of hydrogen is the sum from column I. In cell C89 and D89 I type

$$=SUM(H83:H86) \text{ and } =SUM(I83:I86)$$

The reaction stoichiometry is 1 O₂ per 1 carbon to CO₂ and 0.25 O₂ per 1 hydrogen to H₂O:



I enter these value in cells E89 and F89. The amount of oxygen for complete combustion is:

$$(\text{mol C}) \frac{1 \text{ mol O}_2}{1 \text{ mol C}} + (\text{mol H}) \frac{0.5 \text{ mol O}_2}{2 \text{ mol H}} = \text{mol O}_2$$

In cell G89 I enter the formula:

$$=(C89*E89)+(D89*F89)$$

After adding labels and formatting, the final result is:

	A	B	C	D	E	F	G	H
87								
88			total mol C	total mol H	CO2 stoich	H2O stoich	mol O2	
89			7.10E-03	1.47E-02	1	0.5	1.44E-02	
90			mol	mol	1 O ₂ /1 CO ₂	0.5 O ₂ /H ₂ O	mol	
91							=(C89*E89)+(D89*F89)	

3.B gravimetry

This worksheet has two tables, Table 3.B.1 lists several samples to be analyzed by gravimetry and Table 3.B.2 lists analytical results for a gravimetric analysis. For Table 3.B.1 the exercise is to predict the precipitate weight given the expected analyte concentration. For Table 3.B.2 the results are given and the calculation is to determine the analyte concentration in the unknown sample.

Concepts	Concept Synopsis
gravimetry	Gravimetry, or gravimetric analysis, is a quantitative method to determine an analyte concentration by weighing a pure, solid form of the analyte.

1. Predict the precipitate weight for each case in Table 3.B.1.

First, outline the calculation:

1. use stated concentration to convert g of sample to g of analyte:
(g sample) \rightarrow (g analyte)
2. use formula weight to convert g analyte to mol of analyte:
(g analyte) \rightarrow (mol analyte)
3. use the stoichiometry to convert mol analyte to mol precipitate:
(mol analyte) \rightarrow (mol precipitate)
4. use formula weight to convert mol precipitate to g precipitate:
(mol precipitate) \rightarrow (g precipitate)

First I copy the information in Table 3.B.1 into new cells so that I can use the values in formulas. I include sample amounts in grams and the analyte concentrations as fractions. I assume that the water sample has a density of 1.0 g/mL.

	A	B	C	D	E	F	G
12		Table 3.B.1	sample		analyte	precipitating	
13		sample	weight	analyte	conc	agent	precipitate
14							
15		brass filings	0.1001 g	Cu	60.7%	NH ₄ SCN	CuSCN
16		fertilizer	1.55 g	Mg	11.0 %	(NH ₄) ₂ HPO ₄	MgP ₂ O ₇
17		fertilizer	1.64 g	S	22.0 %	BaCl ₂	BaSO ₄
18		wastewater	250.0 mL	Al ³⁺	122 ppm	succinic acid	Al ₂ O ₃
19							
20							
21		sample	sample amt	fraction			
22		brass filings	0.1001	0.607			
23		fertilizer	1.55	0.11			
24		fertilizer	1.64	0.22			
25		wastewater	250.0	1.22E-04			
26							
27			g				

Multiplying the sample weight by the fraction of the analyte gives the amount of analyte in the sample. For the brass filings, in cell E22 I enter the formula:

$$=C22*D22$$

I type the formula weight of the analyte atoms in column F. Dividing the mass of Cu by the formula weight gives the number of moles of Cu in the sample. In cell G22 I enter the formula:

$$=E22/F22$$

To go from mol of analyte to mol of precipitate, I correct for the stoichiometry of the analyte atom in the precipitate formula. For the brass filings, there is one Cu per each CuSCN. For the wastewater sample, to go from Al to Al₂O₃ I will multiply by 1/2: 1 mol Al₂O₃ per 2 mol Al. I enter stoichiometric factors in column H. In cell I22 I enter the formula:

$$=G22*H22$$

I highlight cells E22, G22, and I22, and copy down for the other samples. After adding labels, units, and highlights, the calculations look like the following:

	A	B	C	D	E	F	G	H	I
20									
21		sample	sample amt	fraction	analyte wt	f.w.	mol analyte	stoich.	mol precip
22		brass filings	0.1001	0.607	0.0608	63.546	0.00095617	1	0.00095617
23		fertilizer	1.55	0.11	0.1705	24.305	0.00701502	0.5	0.00350751
24		fertilizer	1.64	0.22	0.3608	32.065	0.01125214	1	0.01125214
25		wastewater	250.0	1.22E-04	0.0305	26.982	0.00113038	0.5	0.00056519
26									
27			g		g	g/mol	mol		mol
28					=C22*D22		=E22/F22		=G22*H22

Now I can convert the moles of precipitate to weight using the formula weight of the precipitates. I copy the results in column I below the existing table to cells C32:C35 simply for ease of printing. In column D I enter the formula weights of the precipitates. For the brass filings, in cell E32 I type:

=C32*D32

Copying this cell down the column and adding labels and formatting produces something like the following figure:

	A	B	C	D	E	F
30						
31		sample	mol precip	f.w.	predicted wt	
32		brass filings	0.00095617	121.628	0.1163	g CuSCN
33		fertilizer	0.00350751	222.553	0.7806	g Mg ₂ P ₂ O ₇
34		fertilizer	0.01125214	233.390	2.6261	g BaSO ₄
35		wastewater	0.00056519	101.961	0.0576	g Al ₂ O ₃
36						
37			mol	g/mol	g	
38			=I22		=C32*D32	

2. Calculate the total suspended solids (TSS) for the water sample.

Three results are given in Table 3.B.2. For each trial, the tared, or empty, weight of a crucible and filter is given in column C. The other values are the weights of the crucible and sample after drying and cooling until reaching a constant weight. I copy the final weight for each trial to column H. For example, in cell H79 I type =F79. The weight of the collected sample is the final weight minus the tared weight. For trial 1, in cell I79 I enter the formula:

=H79-C79

Copying cell I79 down the next two rows gives something like the following:

	A	B	C	D	E	F	G	H	I
77		Table 3.B.2		crucible/filter/solids to constant weight					
78		trial	tared wt	wt 1	wt 2	wt 3	wt 4	final wt (g)	wt solids (g)
79		1	31.6476	31.6777	31.6555	31.6552		31.6552	0.0076
80		2	31.6116	31.6344	31.6195	31.6192	31.6181	31.6181	0.0065
81		3	32.1148	32.1282	32.1224	32.1222		32.1222	0.0074
82									g
83									=H79-C79

I copy the weight to a new location and convert to mg by multiplying by 1000 mg/g. In cell C87 I type:

$$=I79*1000$$

I copy this cell down two rows for trials 2 and 3. I place the mean and standard deviation of the three weights in cells E87 and E88:

$$=AVERAGE(C87:C89)$$

$$=STDEV(C87:C89)$$

Finally, to find TSS I divide by the volume of solution that I filtered. There were two aliquots of 100 mL each, so in cell G87 I type the volume as 0.200 L. Dividing the weight in mg by this volume gives TSS in mg/L. In cells H87 and H88 I type:

$$=E87/G87$$

$$= E88/G87$$

On adding highlighting my final results looks like the following figure:

	A	B	C	D	E	F	G	H	I
85									
86		trial	wt solids (mg)		solids wt		volume	TSS (mg/L)	
87		1	7.6		7.17	mean	0.200	35.8	mean
88		2	6.5		0.59	± std dev		2.9	± std dev
89		3	7.4						
90			mg		mg		L	mg/L	
91			=I79*1000		=F86/G86			=E85/G85	

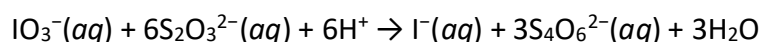
3.C titration

This worksheet contains two tables of titration data. Table A 3.C.1 contains results for titrating a thiosulfate solution with a potassium iodate primary standard. Table A 3.C.2 contains results for titrating an iodine unknown using the standardized thiosulfate solution. The first step is to identify strong versus weak acids and bases. Knowing the nature of each acid or base, you can then determine their relative acidity or basicity.

Concepts	Concept Synopsis
titration	Titration is a quantitative method to determine the concentration of an analyte in solution by reacting it completely with a standardized reagent solution, called the titrant.

1. Determine the concentration of the sodium thiosulfate titrant.

The first "unknown" is a solution of sodium thiosulfate, $\text{Na}_2\text{S}_2\text{O}_3$, which will be used as the titrant in the second titration. The thiosulfate solution is prepared to be approximately 0.1 M and the concentration is determined exactly by titration with potassium iodate, KIO_3 , primary standard. Several reagents are added to the titration solution, but the overall reaction is:



The stoichiometry of the titration reaction shows that 6 mol of thiosulfate ion reacts with one mol of iodate ion. The calculation will use this stoichiometry, the weight of the primary standard, and the volume of thiosulfate titrant to determine the thiosulfate concentration. Outlining the calculation:

1. convert g of primary standard to mol of primary standard:
 $(\text{g KIO}_3) \rightarrow (\text{mol IO}_3^-)$
2. convert mol of IO_3^- to mol of $\text{S}_2\text{O}_3^{2-}$ using the reaction stoichiometry:
 $(\text{mol IO}_3^-)(6 \text{ mol S}_2\text{O}_3^{2-}/1 \text{ mol IO}_3^-) \rightarrow (\text{mol S}_2\text{O}_3^{2-})$
3. determine concentration of $\text{S}_2\text{O}_3^{2-}$ from mol of $\text{S}_2\text{O}_3^{2-}$ and the titration result:
 $(\text{mol S}_2\text{O}_3^{2-})/(\text{vol S}_2\text{O}_3^{2-}) \rightarrow (\text{mol/L S}_2\text{O}_3^{2-})$

I can reference the values in Table 3.C.1 directly, but I need a couple of other values for the calculations outlined above. In cell C27 I type the formula weight of KIO_3 , which is 214.001 g/mol. In cell C28 I type the reaction stoichiometry of $(6 \text{ mol S}_2\text{O}_3^{2-}/1 \text{ mol IO}_3^-)$. I also type labels for a new table for the calculations:

	A	B	C	D	E	F
27		KIO ₃ f.w.	214.001	g/mol		
28		stoichiometry	6	mol thiosulfate/1 mol iodate		
29						
30			mol	mol	vol	conc
31		trial	KIO ₃	Na ₂ S ₂ O ₃	Na ₂ S ₂ O ₃	Na ₂ S ₂ O ₃
32		1				
33		2				
34		3				

I use the formula weight to convert the primary standard weights to moles of KIO₃. For trial 1, I type the following in cell C32:

=C23/\$C\$27

I multiply this value by the reaction stoichiometry to get moles of thiosulfate. In cell D32 I type:

=C32*\$C\$28

The titration results give the volume of thiosulfate solution in mL. In cell E32 I convert to L using:

=D23/1000

The concentration of the thiosulfate is then the number of moles divided by the volume. In cell F32 I type:

=D32/E32

I highlight cells C32:F32 and copy down the next two rows for trials 2 and 3. Taking the average of the three trials gives me the thiosulfate concentration. In cell F36 and F37 I type:

=AVERAGE(F32:F34)

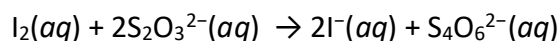
=STDEV(F32:F34)

After highlighting the results look like the following figure:

	A	B	C	D	E	F	G	H
27		KIO ₃ f.w.	214.001	g/mol				
28		stoichiometry	6	mol thiosulfate/1 mol iodate				
29								
30			mol	mol	vol	conc		
31		trial	KIO ₃	Na ₂ S ₂ O ₃	Na ₂ S ₂ O ₃	Na ₂ S ₂ O ₃	titrant conc (M)	
32		1	6.939E-04	0.00416353	0.03852	0.1081	0.1082	mean
33		2	7.075E-04	4.245E-03	0.03914	0.1085	0.0002	std dev
34		3	7.042E-04	4.225E-03	0.03907	0.1081		
35								
36			mol	mol	L	mol/L	mol/L	
37			=C23/\$C\$27	=C32*\$C\$28	=D23/1000	=D32/E32	=AVERAGE(F32:F34)	
38								

2. Determine the concentration of I₂ in the unknown.

Table 3.C.2 gives the results for three trials of a titration of an unknown containing I₂. The titration reaction is:



The stoichiometry of the titration reaction shows that 2 mol of thiosulfate ion reacts with one mol of iodine. The calculation will use this stoichiometry, the volume of thiosulfate titrant, and the volume of unknown solution to determine the I₂ concentration. Outlining the calculation:

1. convert volume of titrant to mol of titrant using the concentration of the titrant:

$$(L S_2O_3^{2-})(mol/L S_2O_3^{2-}) \rightarrow (mol S_2O_3^{2-})$$

2. convert mol of S₂O₃²⁻ to mol of I₂ using the reaction stoichiometry:

$$(mol S_2O_3^{2-})(1 mol I_2/2 mol S_2O_3^{2-}) \rightarrow (mol I_2)$$

3. determine concentration of I₂ by dividing the number of moles by volume:

$$(mol I_2)/(vol I_2) \rightarrow (mol/L I_2)$$

I can reference the values in Table 3.C.2 directly and Question 1 provides the concentration of the thiosulfate titrant in cell F38. In cell C42 I type the reaction stoichiometry of 1/2 (1 mol I₂/2 mol S₂O₃²⁻). I also type labels for a new table for the calculations:

	A	B	C	D	E	F
41		stoichiometry	0.5	mol thiosulfate/1 mol iodine		
42						
43			vol	mol	mol	conc
44		trial	Na ₂ S ₂ O ₃	Na ₂ S ₂ O ₃	I ₂	I ₂
45		a				
46		b				
47		c				

The titration results in Table 3.C.2 give the volume of thiosulfate solution in mL. In cell C45 I convert to L for trial a using:

$$=H23/1000$$

I convert to mol using the concentration of the thiosulfate titrant. For trial a, I type the following in cell D45:

$$=C45*\$G\$32$$

I multiply this value by the reaction stoichiometry to get moles of I₂. In cell E45 I type:

$$=D45*\$C\$41$$

The concentration of the I₂ unknown is then the number of moles divided by the volume. In cell F45 I type:

$$=1000*E45/G23$$

I highlight cells C45:F45 and copy down the next two rows for trials b and c. Taking the average of the three trials as was done in question 1 gives the unknown I₂ concentration. After highlighting the results will look something like the following figure:

	A	B	C	D	E	F	G	H
41		stoichiometry	0.5	mol thiosulfate/1 mol iodine				
42								
43			vol	mol	mol	conc		
44		trial	Na ₂ S ₂ O ₃	Na ₂ S ₂ O ₃	I ₂	I ₂	unknown conc (M)	
45		a	2.299E-02	2.488E-03	1.244E-03	4.976E-02	0.04951	mean
46		b	2.291E-02	2.480E-03	1.240E-03	4.959E-02	0.00030	std dev
47		c	2.272E-02	2.459E-03	1.229E-03	4.918E-02		
48								
49			L	mol	mol	mol/L	mol/L	
50			=H23/1000	=C45*\$G\$32	=D45*\$C\$41	=1000*E45/G23	=AVERAGE(F45:F47)	

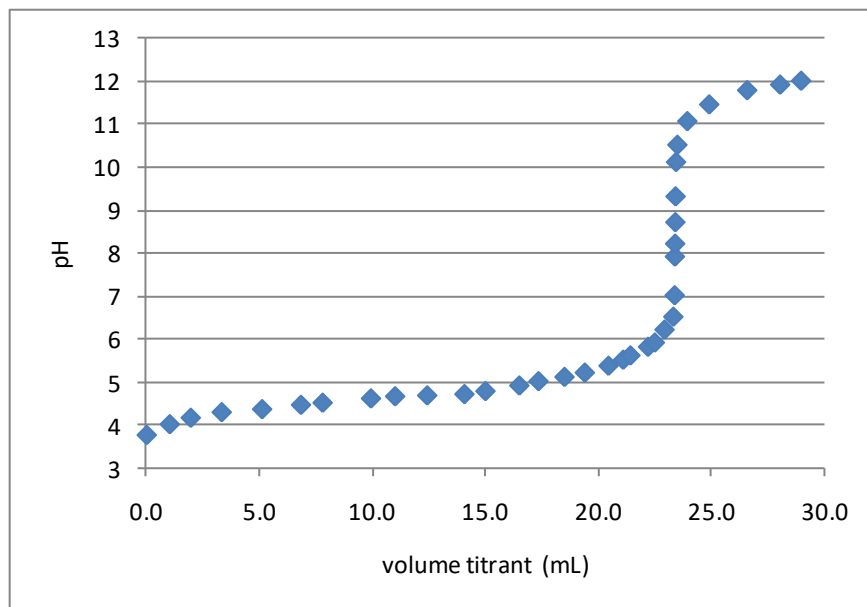
3.D titration-curves

This worksheet contains data of the titration of vinegar, which contains acetic acid, with NaOH titrant. The exercise is to plot the data to determine the end point. The concentration of acetic acid in the sample is determined from the experimental end point.

Concepts	Concept Synopsis
titration curve	A plot of an analytical signal versus titrant volume to determine an end point.

1. Insert a scatter chart to plot the data as pH versus titrant volume.

Highlight the titration data in Table 3.D.1. Click on the Insert ribbon and select the scatter chart. After adjusting the axes and entering labels to your liking, the plot will look something like the following figure:



2. Generate a Gran plot of the data.

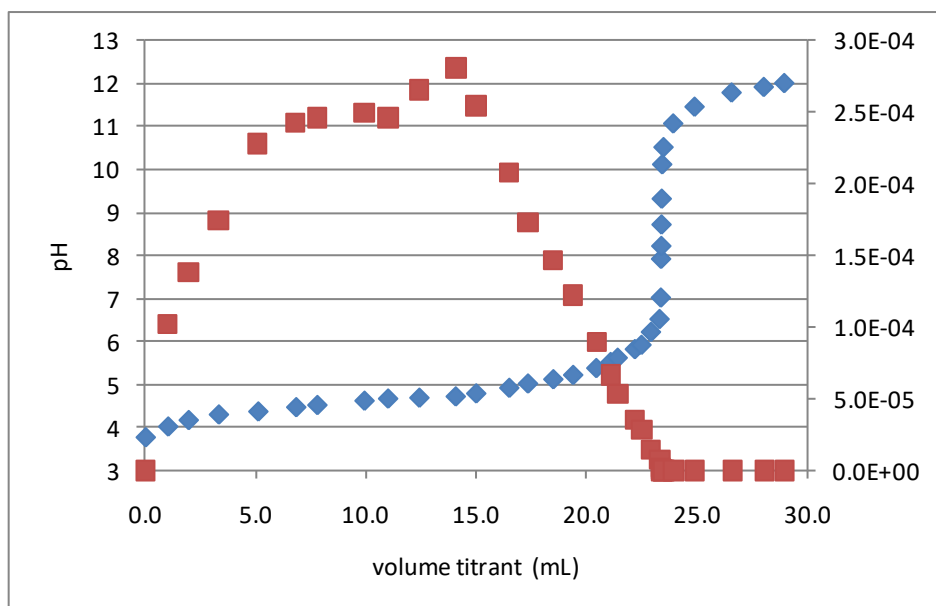
The Gran plot uses the following expression:

$$V_{\text{titrant}} \times 10^{-\text{pH}}$$

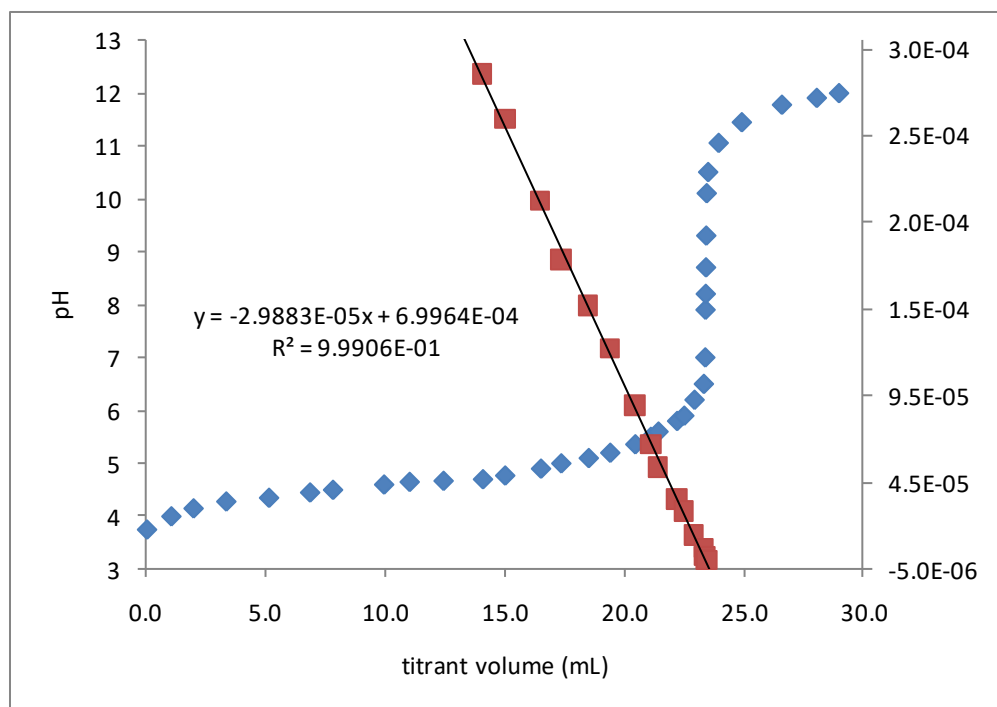
Plotting this expression versus V_{titrant} will generate a line that extrapolates to the end point value. In cell D19 type:

$$=B19*10^{-C19}$$

Click on this cell and double click the lower right handle to copy down the column. With the data still selected, press Ctrl-C, click on the chart, and press Ctrl-V to plot the data. The new curve will not be visible if you have the y axis set as in the figure above. Change the value in D19 to 6 or 7 so you can see it on the chart. Right click on the data point that you can see and select Format Data Series... Choose Secondary axis and click the close button. Now a new y axis will appear on the right side of the chart. Change the value in D19 back to zero. Adjust the formatting of the secondary axis to your liking.



The early and later points are not useful and we will use only the linear range. Delete the points for less than 14 mL of titrant. The later points are harder to see, so right-click on a data point on the chart and add a trendline. Select both 'Display Equation on chart' and 'Display R-squared value on chart' and click the Close button. Delete the higher values to obtain the maximum R-squared value. The result will be something like the following figure:



We will use the linear equation in the next question to find the end point.

3. Determine the concentration of the acid in the unknown solution.

The x-intercept of the Gran plot gives us the end point. I find the slope and intercept of the data by typing in cells G29 and G30:

=SLOPE(D19:D53,B19:B53)
 =INTERCEPT(D19:D53,B19:B53)

I include the full range for the data even though I've deleted many of the y values. If I add values back in the formulas will still work. The x-intercept is:

=-G30/G29

The results are as follows, the slope and intercept values are the same as from the trendline:

slope:	-2.988E-05	
intercept:	0.00069964	
x-intercept:	23.413	mL

I use the endpoint from the Gran plot to determine the unknown. I type the concentration of the NaOH titrant, 0.2550 M, in cell G33. I copy the titrant volume to cell G34 and convert to L by dividing by 1000. Multiplying the titrant concentration by the titrant volume gives me moles of OH^- . In cell G35 I type:

=G33*G34

The moles of H^+ is equal to moles of OH^- . In cell G36 I enter:

=G35

This step is unnecessary, but it gives me a placekeeper in case I adapt this worksheet to a titration where the stoichiometry is different from 1:1. In cell G37 I type the sample volume of 0.01000 L. The unknown concentration is the moles of divided by the sample volume. In cell G38 I type:

=G35/G37

After adding highlighting the results look something like the following figure:

	A	B	C	D	E	F	G	H
17		Table 3.D.1						
18		mL titrant	pH					
19		0.00	3.75					
20		1.02	4.00					
21		1.95	4.15					
22		3.32	4.28					
23		5.11	4.35					
24		6.83	4.45					
25		7.79	4.50					
26		9.93	4.60					
27		11.00	4.65					
28		12.42	4.67					
29		14.07	4.70	0.00028073		slope:	-2.988E-05	
30		15.00	4.77	0.00025474		intercept:	0.00069964	
31		16.50	4.90	0.00020772		x-intercept:	23.413	mL
32		17.35	5.00	0.0001735				
33		18.50	5.10	0.00014695		titrant conc:	0.2550	M NaOH
34		19.40	5.20	0.00012241		titrant vol:	0.0234	L
35		20.45	5.36	8.9267E-05		mol OH:	0.0060	mol
36		21.10	5.50	6.6724E-05		mol H:	0.0060	mol
37		21.42	5.60	5.3805E-05		sample vol:	0.0100	
38		22.20	5.80	3.5185E-05		sample conc:	0.5970	mol/L
39		22.50	5.90	2.8326E-05				
40		22.93	6.20	1.4468E-05				
41		23.32	6.50	7.3744E-06				
42		23.38	7.00	2.338E-06				
43		23.39	7.90	2.9446E-07				
44		23.40	8.20	1.4764E-07				
45		23.41	8.70	4.6709E-08				
46		23.42	9.30	1.1738E-08				
47		23.44	10.10	1.8619E-09				
48		23.50	10.50					
49		23.94	11.05					
50		24.91	11.44					
51		26.59	11.77					
52		28.05	11.90					
53		28.98	11.99					