Experiment 2 (part b) results sheet (*Make sure that you paste this results sheet into your lab notebook)*

Concentration of sodium hydroxide (M)	0.100 M
Prepared benzoic acid derivative	2-Methylbenzoic acid
Assigned benzoic acid derivative	4-Methylbenzoic acid

Group Results

Acid	pKa
2-Methylbenzoic acid	
2-Methoxybenzoic acid	5.2
Benzoic acid	5.2
4-Methylbenzoic acid	
4-Methoxybenzoic acid	5.3
2-Hydroxybenzoic acid	3.6

Table 1: Titration of benzoic acid derivative 2-Methylbenzoic acid with NaOH with more data points near equivalence & half-equivalence points

Reading	Burette reading (mL)	pH
0	0.0	2.98
1	1.0	3.57
2	2.0	3.90
3	3.0	4.12
4	4.0	4.29
5	5.0	4.44
6	6.0	4.55
7	7.0	4.66
8	8.0	4.77
9	9.0	4.88
10	9.1	4.89
11	9.2	4.90
12	9.3	4.91
13	9.4	4.92
14	9.5	4.93
15	9.6	4.94
16	9.7	4.95
17	9.8	4.96
18	9.9	4.97
19	10.0	4.98
20	10.1	4.99
21	10.2	5.00
22	10.3	5.02
23	10.4	5.03
24	10.5	5.04
25	11.5	5.13
26	12.5	5.25
27	13.5	5.38
28	14.5	5.51
29	15.5	5.65
30	16.5	5.87
31	17.5	6.13
32	17.6	6.16
33	17.7	6.21
34	17.8	6.25
35	17.9	6.29
36	18.0	6.35
37	18.1	6.41
38	18.2	6.45
39	18.3	6.52
40	18.4	6.59
41	18.5	6.67
42	18.6	6.72
43	18.7	6.91
44	18.8	7.05
45	18.9	7.20
46	19.0	7.52
47	19.1	7.83
48	19.2	10.90
49	19.3	11.17
50	19.4	11.43
51	19.5	11.58
52	19.6	11.79
53	19.7	11.83
54	19.8	11.92
55	19.9	11.97
56	20.0	12.03
57		
58		
59		
60		
61		
62		
63		
64		

Table 2: Titration of benzoic acid derivative 4-Methylbenzoic acid with NaOH with more data points near equivalence & half-equivalence points

Reading	Burette reading (mL)	pH
0	0.0	3.11
1	1.0	3.78
2	2.0	4.13
3	3.0	4.35
4	4.0	4.52
5	5.0	4.67
6	6.0	4.80
7	7.0	4.91
8	8.0	5.02
9	8.1	5.03
10	8.2	5.04
11	8.3	5.05
12	8.4	5.06
13	8.5	5.07
14	8.6	5.08
15	8.7	5.09
16	8.8	5.10
17	8.9	5.11
18	9.0	5.12
19	9.1	5.13
20	9.2	5.14
21	9.3	5.15
22	9.4	5.16
23	9.5	5.18
24	9.6	5.19
25	9.7	5.2
26	9.8	5.21
27	9.9	5.22
28	10.0	5.23
29	10.1	5.24
30	10.2	5.24
31	10.3	5.26
32	10.4	5.26
33	10.5	5.27
34	10.6	5.28
35	10.7	5.3
36	10.8	5.31
37	10.9	5.32
38	11.0	5.33
39	12.0	5.44
40	13.0	5.57
41	14.0	5.70
42	15.0	5.85
43	16.0	6.04
44	17.0	6.29
45	18.0	6.72
46	18.1	6.78
47	18.2	6.86
48	18.3	6.96
49	18.4	7.03
50	18.5	7.17
51	18.6	7.29
52	18.7	7.59
53	18.8	8.52
54	18.9	9.82
55	19.0	10.64
56	19.1	10.86
57	19.2	11.03
58	19.3	11.15
59	19.4	11.23
60	19.6	11.29
61	19.7	11.33
62	19.8	11.34
63	19.9	11.34
64	20.0	11.35

Calculating pK$_a$ using Excel

1. Set up the following table in Excel, with column headings from A1 to J1.

	A	B	C	D	E	F	G	H
1	Volume reading (mL)	Titration volume (mL)	pH	ΔV	ΔpH	$\Delta pH/\Delta V$	V(ave)	$\Delta(\Delta pH)/\Delta V^2)$

2. Fill in the volume reading and pH values.

	A	B	C	D	E	F	G	H
1	Volume reading (mL)	Titration volume (mL)	pH	ΔV	ΔpH	$\Delta pH/\Delta V$	V(ave)	$\Delta(\Delta pH)/\Delta V^2)$
2	*From results sheet*		*From results sheet*					
3	*From results sheet*		*From results sheet*					

3. Into rows 2 and 3, fill in the following values and formulae, substituting **CONC** with the concentration of sodium hydroxide solution. Here you are using the finite difference method to calculate $\Delta pH/\Delta V$ as an approximation to the actual derivative or gradient of your titration curve. Likewise for the second derivative.

	A	B	C	D	E	F	G	H
1	Volume reading (mL)	Titration volume (mL)	pH	ΔV	ΔpH	$\Delta pH/\Delta V$	V(average)	$\Delta(\Delta pH)/\Delta V^2)$
2	*From results sheet*	0	*From results sheet*	=B3-B2	=C3-C2	=E2/D2	=(B3+B2)/2	=(F3-F2)/(G3-G2)
3	*From results sheet*	=A3-A$2	*From results sheet*	=B4-B3	=C4-C3	=E3/D3	=(B4+B3)/2	=(F4-F3)/(G4-G3)

4. Fill down the formulae for columns B, D, E, F, G and H. To do this, click on a cell with the formula in it. Hover over the square in the bottom right-hand corner of the square – a cross should appear. Click, and drag down the columns to the lowest cell you want to fill.

5. Use Excel to draw <u>three</u> graphs (i) pH vs Titration volume; (ii) $\Delta pH/\Delta V$ vs average titration volume, V(average), and (iii) $\Delta(\Delta pH)/\Delta V^2)$ vs V(average) (volume should be on the x-axis for each graph). The equivalence point is the titration volume where the pH changes most rapidly (steeply) with added NaOH. How does this look on each of your three graphs? Find the equivalence point, and determine which graph gives you the most reliable value. Use this to calculate the half-equivalence point.

6. From column B, find the volume reading closest to the half-equivalence point. Read across to the pH. This is your pK$_a$. (If you have data points equally spaced on either side of the half-equivalence point, you can take their average to determine the pK$_a$.)

7. How accurate is your pK$_a$ determination? You need to consider what factors will determine (i) the uncertainty in your equivalence point and (ii) the uncertainty in your pH measurement, σ_{pH}.

    a. Rate the following factors in order of importance for how much they affect the error in the equivalence point.

      [NaOH]   mass of substituted benzoic acid   volume of ethanol and water for acid solution

           purity of your substituted benzoic acid   titration volume at equivalence point

    Use this to determine (or at least estimate) the error in your half-equivalence point,

      $\sigma_{V/2} = $ $\pm$ mL

    b. What is the uncertainty in an individual pH measurement? i.e. To how many decimal places could you read an individual pH? Were any digits fluctuating? Did the pH readings drift during the experiment? How reproducible was a repeat measurement of the same solution?

        Use this to estimate σ_{pH} = $\pm$.

Suppose first that only the error in volume is important. How much would the pK$_a$ you read as a pH from the data table be affected if you replace $V/2$ with $(V/2 + \sigma_{V/2})$ or $(V/2 - \sigma_{V/2})$? Because the pH is changing slowest near the half-equivalence point (it's buffering the solution), small errors in $V/2$ should not affect the pH much. Therefore they don't usually create big errors in pK$_a$.

Now you can decide what has the bigger effect on your pK$_a$ determination, reading the pH meter or the titration accuracy. Use this to determine the uncertainty on your pK$_a$, and then decide how many digits are significant.