Creating a Hammett Plot in Excel

These instructions will tell you how to do all the calculations and plotting in Excel. You can also elect to do the math by hand using a calculator. That's your choice, either is fine. However, plots must be made in software, not hand-drawn.

1. Create a spreadsheet in Excel that mirrors the data table in the report template. A screenshot of Michelle's excel sheet is below.

	A	B	C	D	E	F	G
1	**Compound**	**Ketone**	**Benzaldehyde**	**σ_p**	**Average time (s)**	**k_{eff} (s^{-1})**	**log(k_{eff}/k_H)**
2	A	Acetone	benzaldehyde				
3	B		p-tolualdehyde				
4	C		p-methoxybenzaldehyde				
5	D		p-chlorobenzaldehyde				
6	E	Cyclohexanone	benzaldehyde				
7	F		p-tolualdehyde				
8	G		p-methoxybenzaldehyde				
9	H		p-chlorobenzaldehyde				
10							

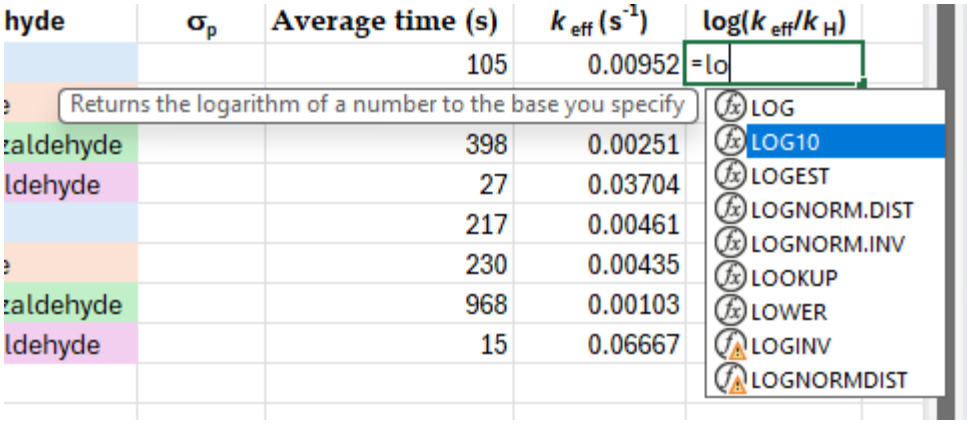
2. Fill in the σ_P values (you can find them in the lab manual)
3. You will have a class data set of the time to precipitate formation. Each compound will have two times reported, since the experiment was run in duplicate. Take the average of these two times for each of the 8 compounds and add them to your Excel sheet.
4. We will calculate the effective rate constant by calculating 1/time for each compound. You can do this by typing "=1/" and then clicking on the cell that the time is in, and hitting enter:

	A	B	C	D	E	F	G
1	**Compound**	**Ketone**	**Benzaldehyde**	**σ_p**	**Average time (s)**	**k_{eff} (s^{-1})**	**log(k_{eff}/k_H)**
2	A	Acetone	benzaldehyde		105	=1/E2	
3	B		p-tolualdehyde				

5. You can make the whole column follow that same formula by clicking that cell, then dragging the green square in the bottom right corner down so that the whole column is contained in the green box.

	A	B	C	D	E	F	G
1	**Compound**	**Ketone**	**Benzaldehyde**	**σ_p**	**Average time (s)**	**k_{eff} (s^{-1})**	**log(k**
2	A	Acetone	benzaldehyde		105	0.00952	
3	B		p-tolualdehyde		108		
4	C		p-methoxybenzaldehyde		398		
5	D		p-chlorobenzaldehyde		27		
6	E	Cyclohexanone	benzaldehyde		217		
7	F		p-tolualdehyde		230		
8	G		p-methoxybenzaldehyde		968		
9	H		p-chlorobenzaldehyde		15		
10							

6. Now you can calculate log(k_{eff}/k_H). Get the formula started by typing "=log" and the following option should appear:



7. Choose LOG10 and then complete the formula as follows. Where the cell for k_H is input, you will need to add the dollar signs ($) to 'lock' the R=H k_{eff} as k_H. Hit enter once you have the formula typed in.

	A	B	C	D	E	F	G
1	Compound	Ketone	Benzaldehyde	σp	Average time (s)	k eff (s-1)	log(k eff/k H)
2	A	Acetone	benzaldehyde		105	0.00952	=LOG10(F2/F2)
3	B		p-tolualdehyde		108	0.00926	
4	C		p-methoxybenzaldehyde		398	0.00251	
5	D		p-chlorobenzaldehyde		27	0.03704	

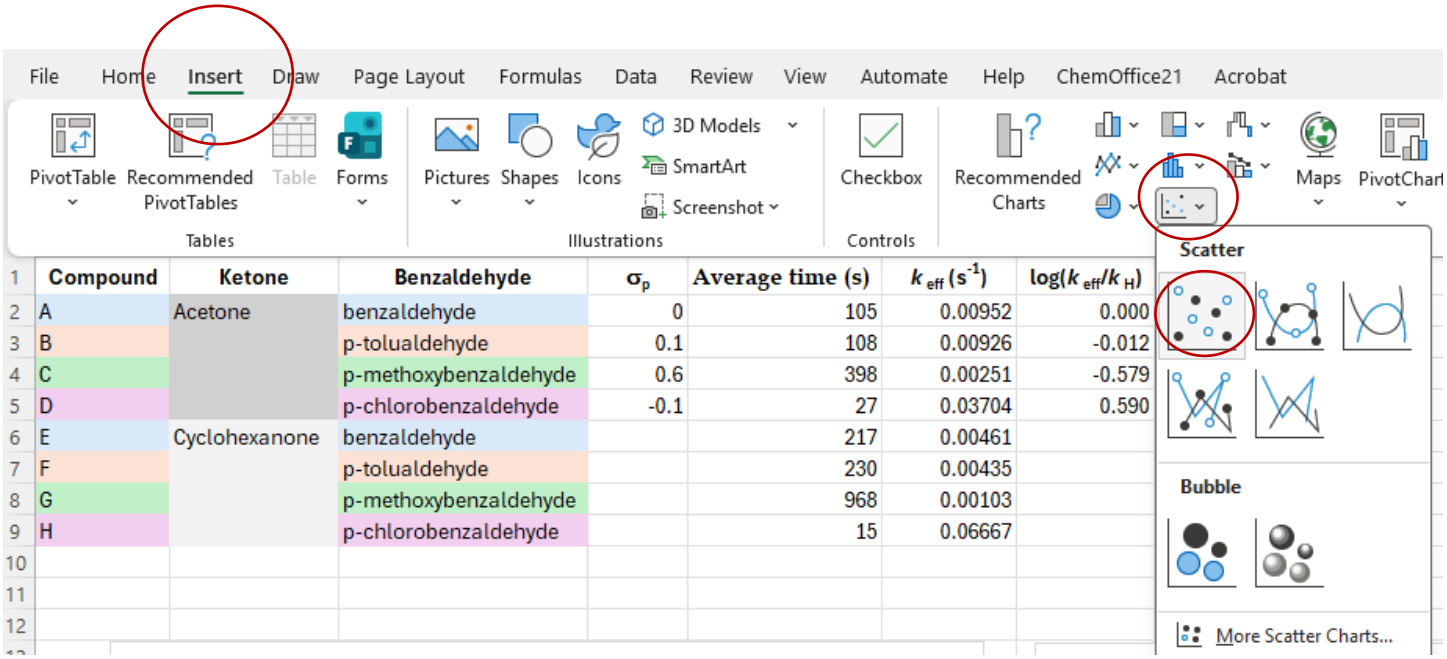
8. Use the green square to extend this formula to all of the compounds A-D, but NOT E-H! k_H for acetone is different than for cyclohexanone.

	A	B	C	D	E	F	G
1	Compound	Ketone	Benzaldehyde	σp	Average time (s)	k eff (s-1)	log(k eff/k H)
2	A	Acetone	benzaldehyde		105	0.00952	0.000
3	B		p-tolualdehyde		108	0.00926	
4	C		p-methoxybenzaldehyde		398	0.00251	
5	D		p-chlorobenzaldehyde		27	0.03704	
6	E	Cyclohexanone	benzaldehyde		217	0.00461	
7	F		p-tolualdehyde		230	0.00435	
8	G		p-methoxybenzaldehyde		968	0.00103	
9	H		p-chlorobenzaldehyde		15	0.06667	

9. Repeat this process for E-F, setting compound E's k_{eff} as the 'locked' k_H for the second set of data.
10. Now we will make the first plot. Click and drag to highlight the cells containing the σ_P values for compounds A-D. There should be a green box around them now. Hold down the shift key and also click and drag to highlight the cells containing $\log(k_{eff}/k_H)$ for compounds A-D. Should look like my example below, but I used fake σ_P values (so don't copy them!).

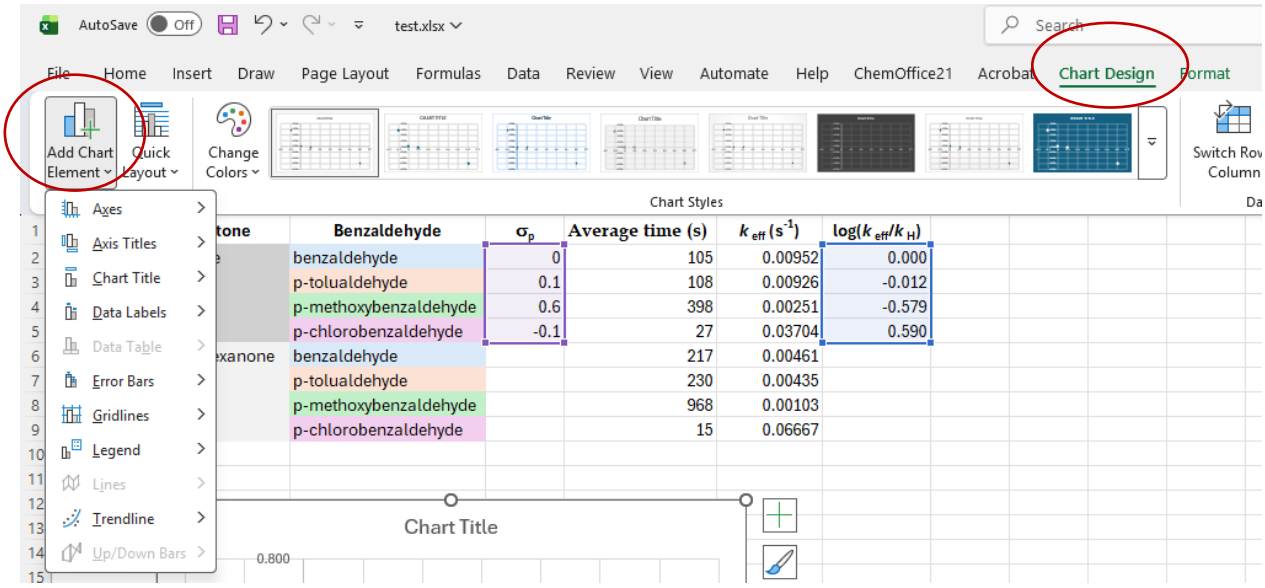
Benzaldehyde	σp	Average time (s)	k eff (s-1)	log(k eff/k H)
benzaldehyde	0	105	0.00952	0.000
p-tolualdehyde	0.1	108	0.00926	-0.012
p-methoxybenzaldehyde	0.6	398	0.00251	-0.579
p-chlorobenzaldehyde	-0.1	27	0.03704	0.590

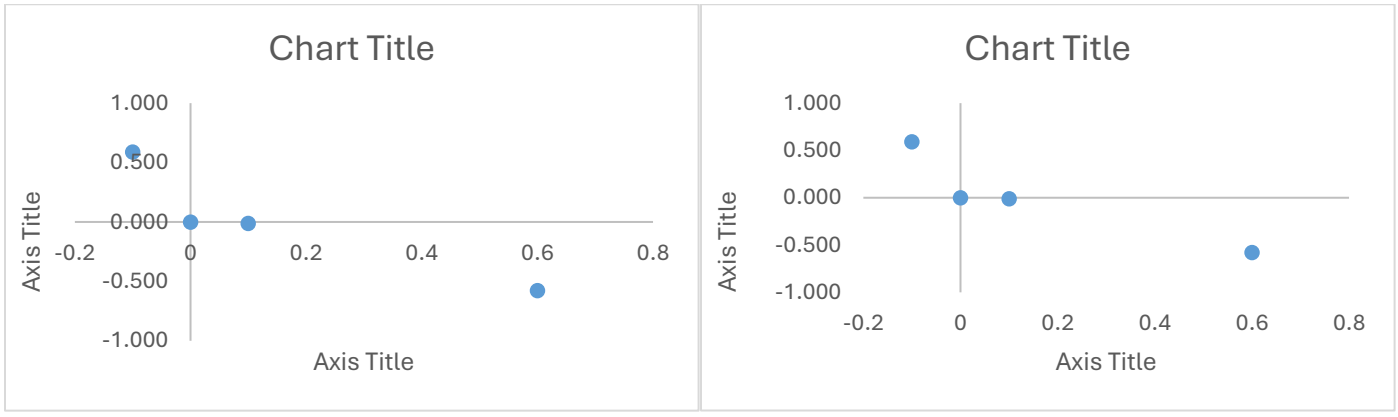
11. Now, click the 'Insert' menu at the top of Excel, find the 'Charts' submenu, and click the scatter plot option. Pick the one that is just points with no line. A plot should appear.



	Compound	Ketone	Benzaldehyde	σ_p	Average time (s)	k_{eff} (s^{-1})	$\log(k_{eff}/k_H)$
2	A	Acetone	benzaldehyde	0	105	0.00952	0.000
3	B		p-tolualdehyde	0.1	108	0.00926	-0.012
4	C		p-methoxybenzaldehyde	0.6	398	0.00251	-0.579
5	D		p-chlorobenzaldehyde	-0.1	27	0.03704	0.590
6	E	Cyclohexanone	benzaldehyde		217	0.00461	
7	F		p-tolualdehyde		230	0.00435	
8	G		p-methoxybenzaldehyde		968	0.00103	
9	H		p-chlorobenzaldehyde		15	0.06667	

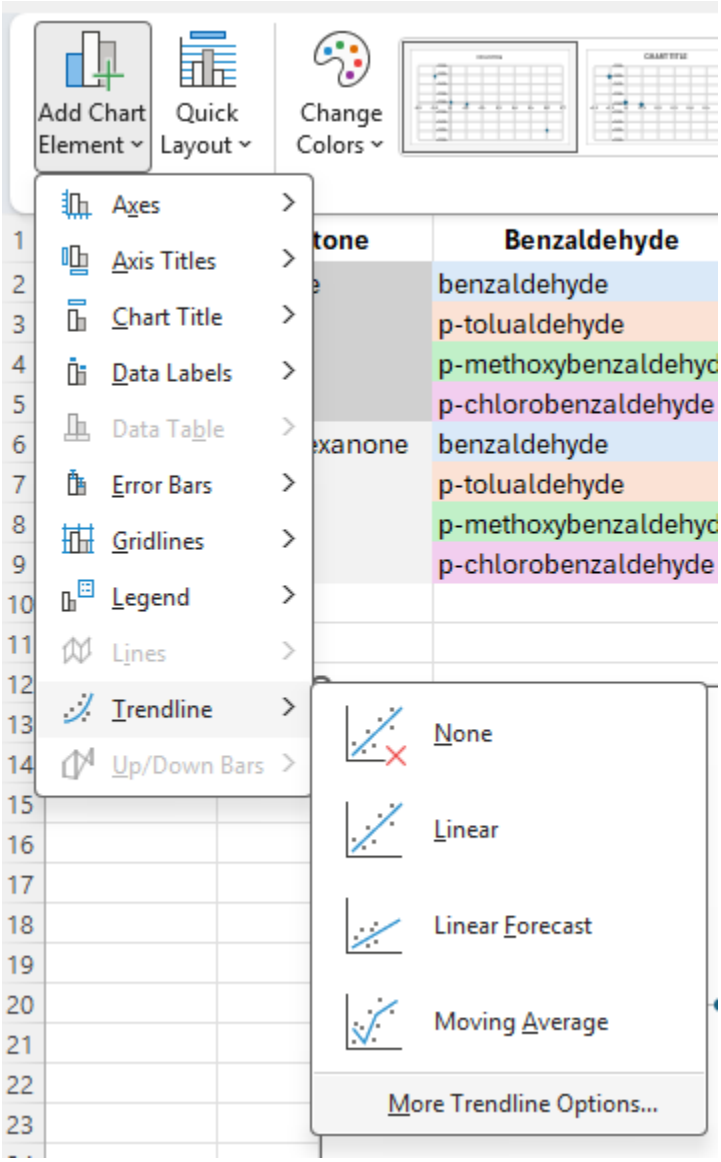
12. Click on the chart, then navigate to the Chart Design tab. The 'Add Chart Element' drop-down will let you add or remove parts of the chart. You are required to have axis titles on both the horizontal and vertical axes, and a chart title. I like to remove gridlines but that is a personal preference. Toggle the chart elements on/off so that your chart has the required features and looks how you want it to.

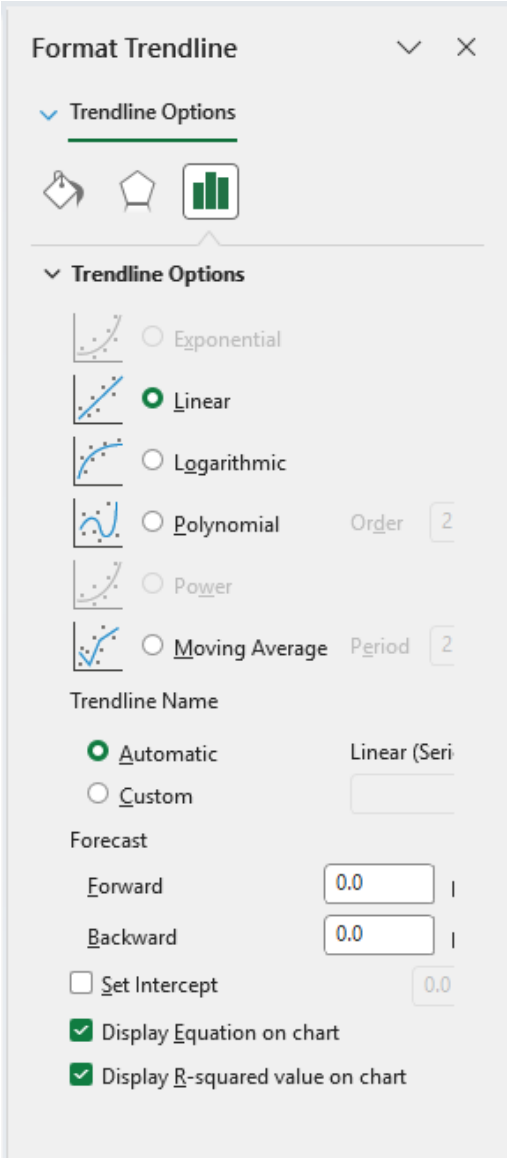




Feel free to move where the axes and numbers are located. Both of the above charts are acceptable.

13. Add a trendline to the chart from the Add Chart Element menu by selecting Trendline and then More Trendline Options. This will open the Format Trendline panel where you can select Linear, Display Equation on chart, and Display R-squared value on chart.





14. Position the resulting line equation and R-squared value so they are legible, make sure your titles are correct, and your Hammett plot should be ready to paste into your report.
15. Do this all again for the cyclohexanone reactions (compounds E-H). 😊