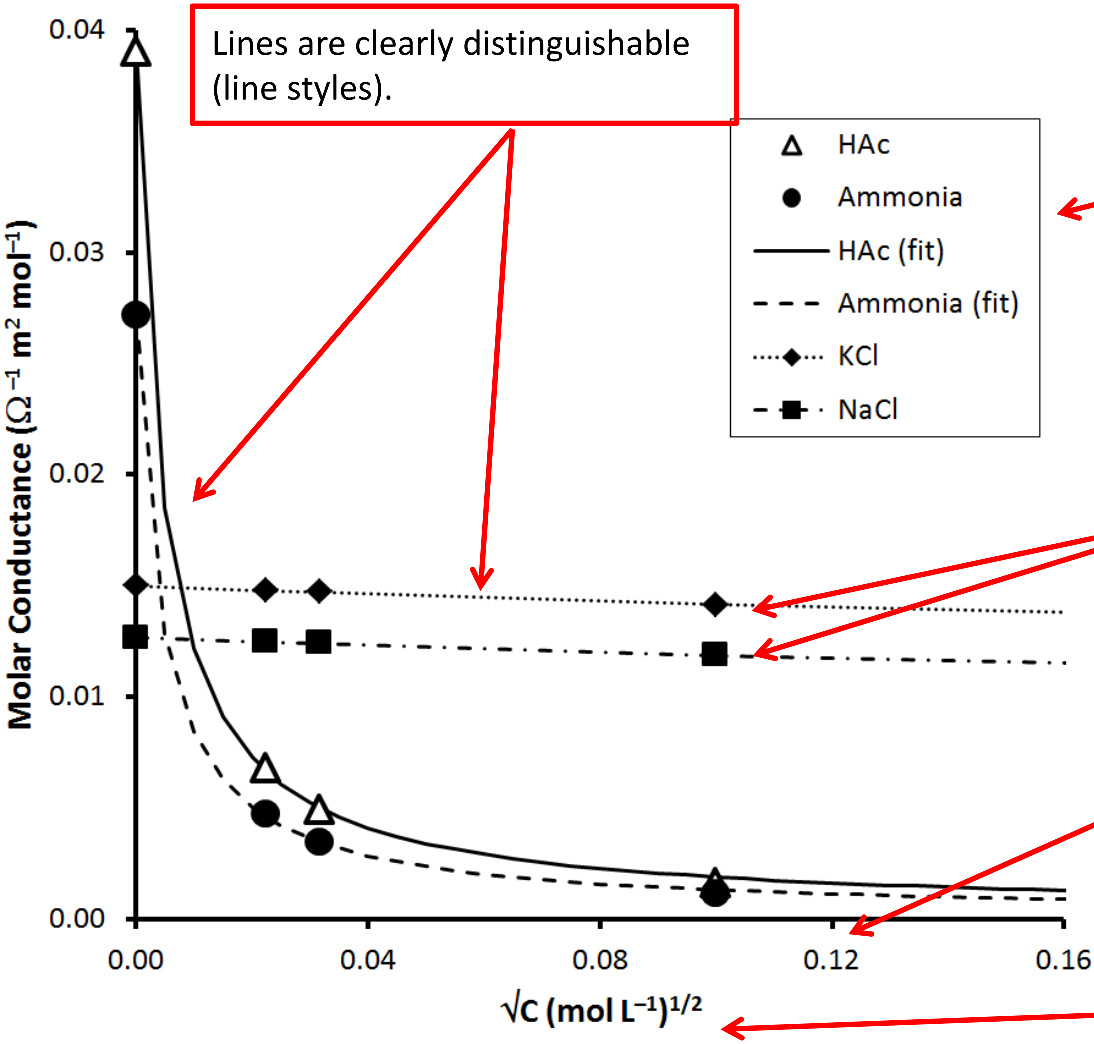
Figures, Figure Captions, and Tables

B. Ramu Ramachandran

Essential aspects of a good figure



The legend (if provided) is placed well (does not obscure data), easily readable (font size) and understandable in the context of the work.

Symbols are different and of appropriate size.

Axis numbering is appropriate (number format, intervals, significant figures, size) and axis range is chosen according to the range of data (both axes).

Axis labels are clear, large enough, and units are provided (if necessary).

Figure 1. The variation of molar conductances of strong and weak electrolytes with concentration.

Concise but descriptive figure caption.

How about this?

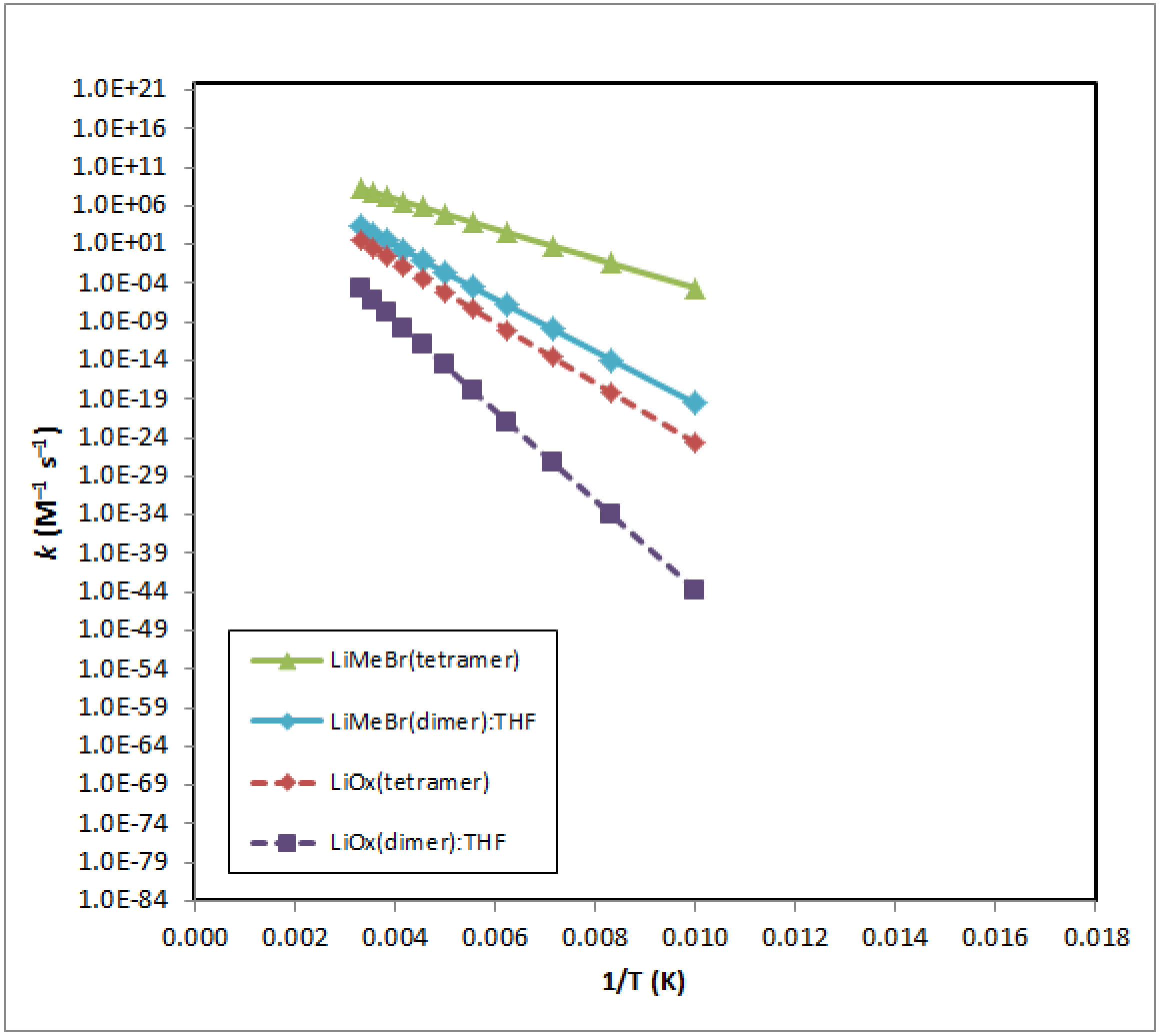


Figure 9. Reaction rate constants.

- Too much wasted space. Ranges of both axes need to be adjusted.
- Numbering of the axes are too dense.
- The figure caption is too terse and unhelpful.
- **Ramu's law:** It should possible to read the abstract of a paper and all figure captions to get a rough idea of what was done and what was found.

Essential aspects of a good figure caption

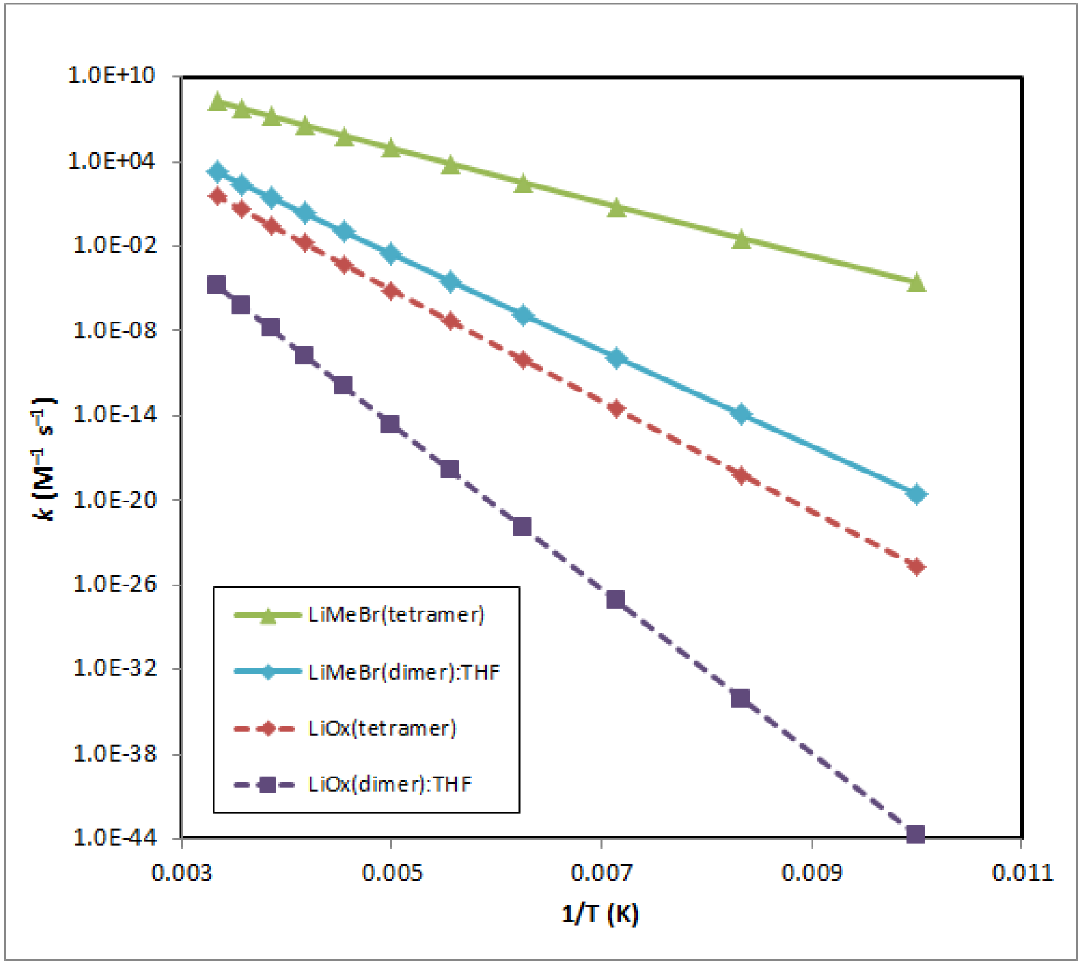


Figure 9. Rate constants for the reactions of bromomethyllithium species and oxiranyllithium species with ethylene in nonpolar media and THF, as a function of temperature.

Figure caption should "explain" the figure.

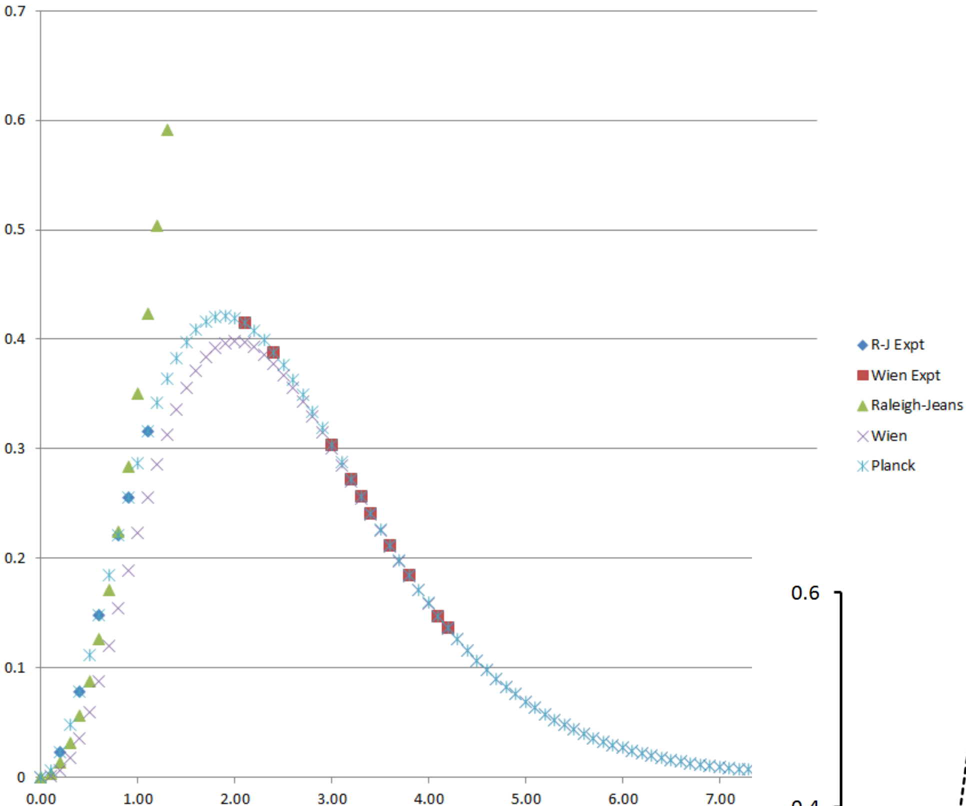
Color should be used only if it is really necessary. This graph actually could be drawn in black & white without any loss of information.

Why not use color everywhere?
Stay tuned.
(Some day we will.)

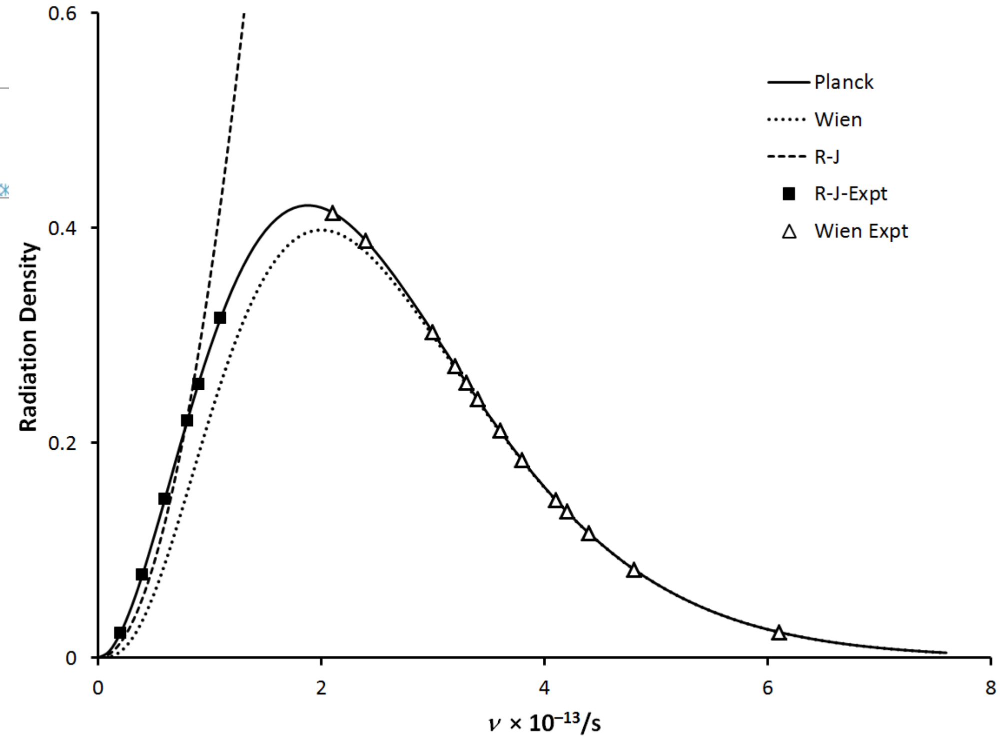
Essential aspects of a good figure

(for black & white reproduction)

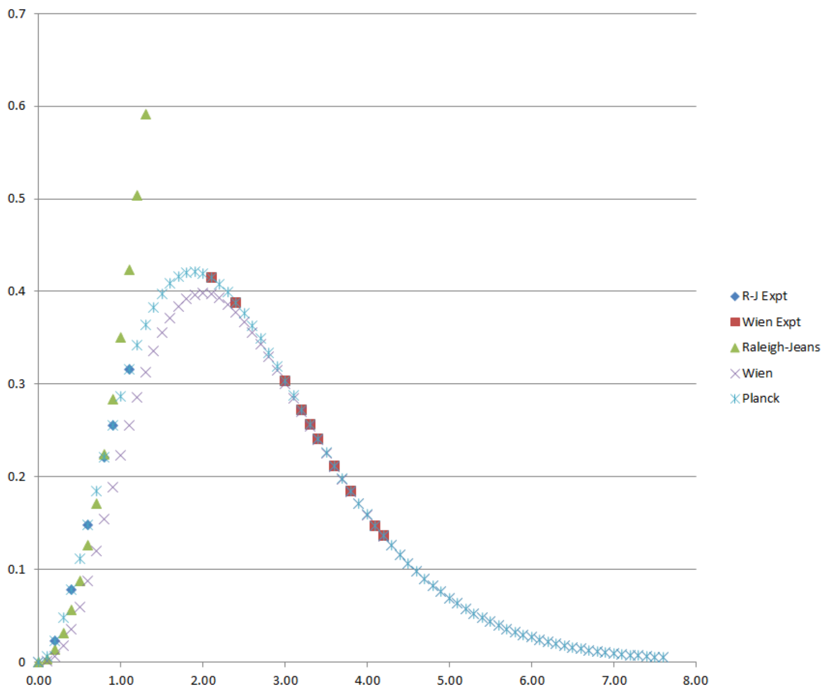
- Majority of figures in scientific journals are black & white.
- Also, majority of available printers/ copiers give you b&w output.
- So, <u>if color is not absolutely essential</u>, it is actually good practice to design your figure for b&w reproduction.
- Excel is probably the most commonly used plotting package. It produces color graphs by default. Default Excel graphs would not be acceptable for publication in most respectable journals.
- The example on the next slide shows the “default” produced by Excel and the changes made to go from there to something we (and most journal editors) can live with.

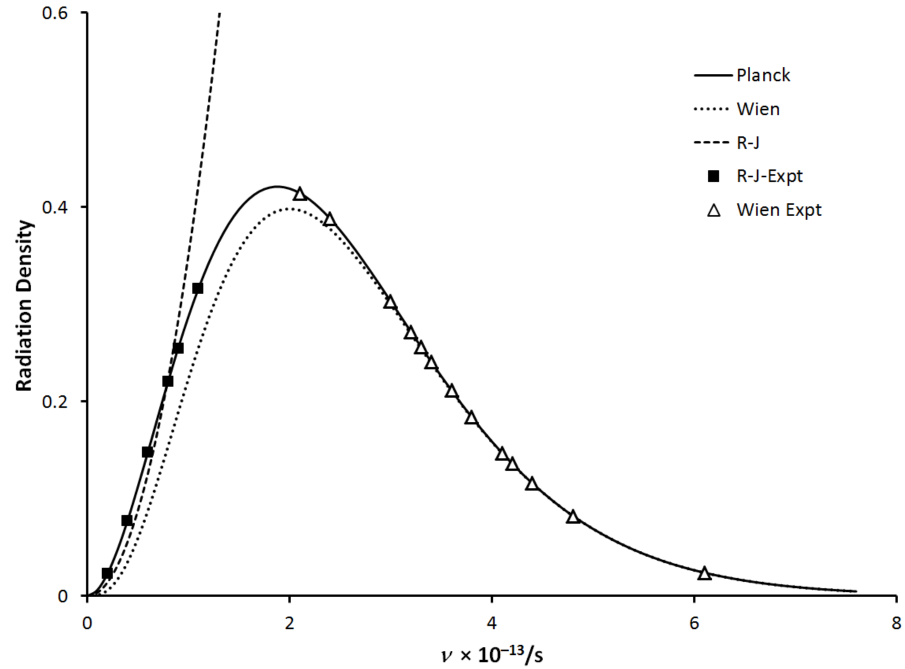


Excel defaults



A more acceptable figure





Problems with Excel defaults (from my PoV)

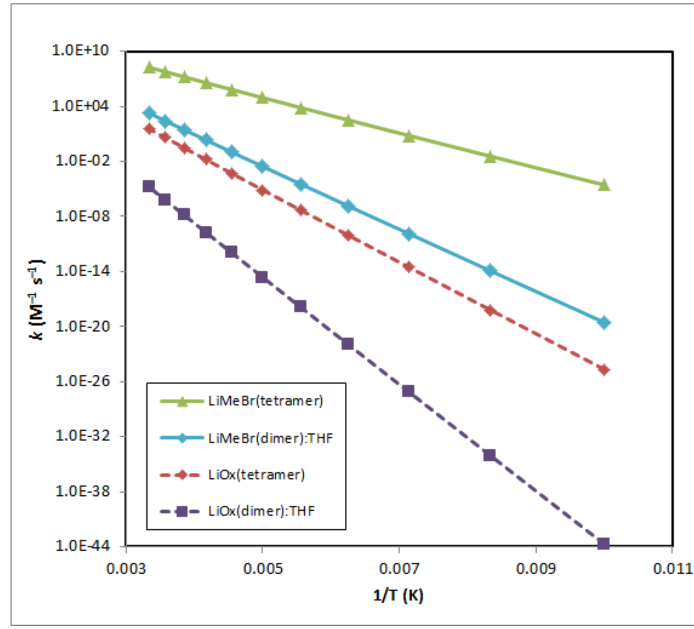
1. Grid lines.
2. Numbering too small.
3. Legend off to one side (not making optimal use of space), font too small.
4. Everything –even related data sets– is shown as symbols without connecting lines.
5. No axis labels. Axis line is too thin and the color is gray.
6. Nothing is gained by extending the vertical axis to 0.7.
7. There is no need for consecutive numbers on axes: 1,2,3,… or 0.1, 0.2, 0.3, … Also, unnecessary decimal places in the X-axis numbers. [It is recommended that numbers are spaced by 2, 5, or 10 (or multiples) depending on the range covered.]
8. Colors are faint and may not copy well on a b&w copier.

Changes made:

1. Turned off grid lines.
2. Increased numbering size.
3. Legend overlaps with figure, makes better use of space and allows the figure itself to be enlarged without occupying more space. Enlarged the font.
4. Theoretical predictions (Raleigh-Jeans, Wien, Planck) are shown as lines without symbols while experimental data collected to verify the R-J and Wien theories are shown as symbols without lines.
5. Axis labels provided. Axis lines made thicker and black.
6. Vertical axis upper limit restricted. (Could restrict to 0.5 without loss of information.)
7. Axis numbering now follows the “2,5,10” rule and unnecessary decimal places have been eliminated.
8. There is really nothing gained by using color in this graph. So, everything is in b&w.

Limitations of Excel

- As we saw in the previous slides, many short-comings of Excel as a plotting package can be overcome by rejecting the defaults.
- However, some limitations are much harder or impossible to overcome.
- Example: When plotting log-scale axes (as in the top figure), it is more professional to show the vertical axis numbers as powers of 10 (as shown to the right). However, Excel cannot do this.
- The graph on the bottom right was produced using PSI-Plot, a very simple and user-friendly (but not free) plotting package.



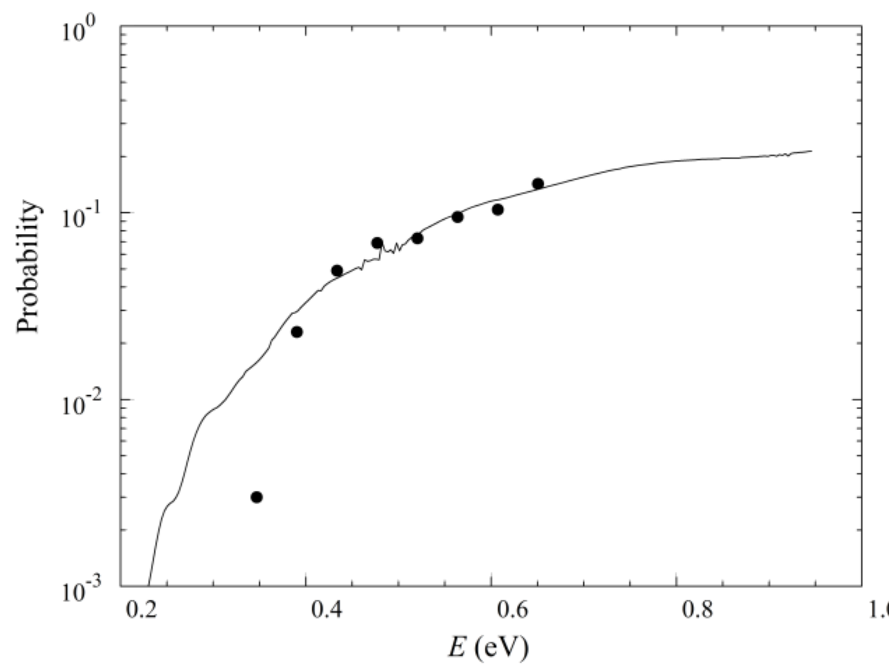
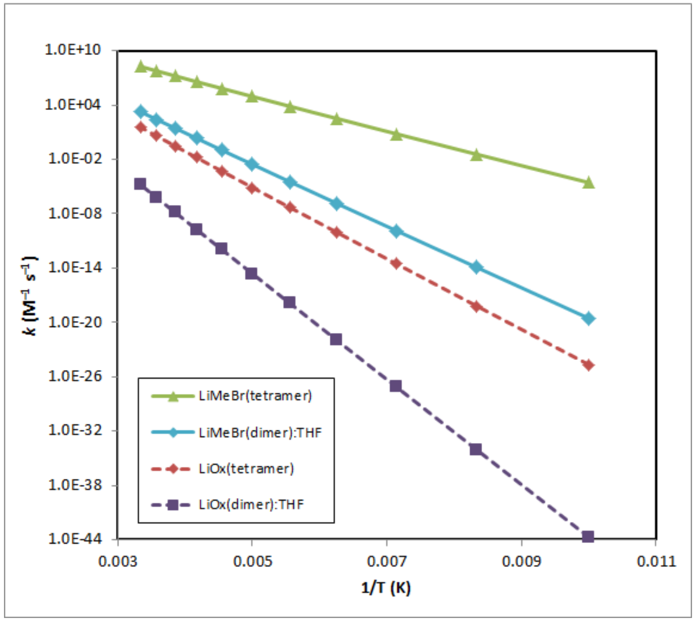
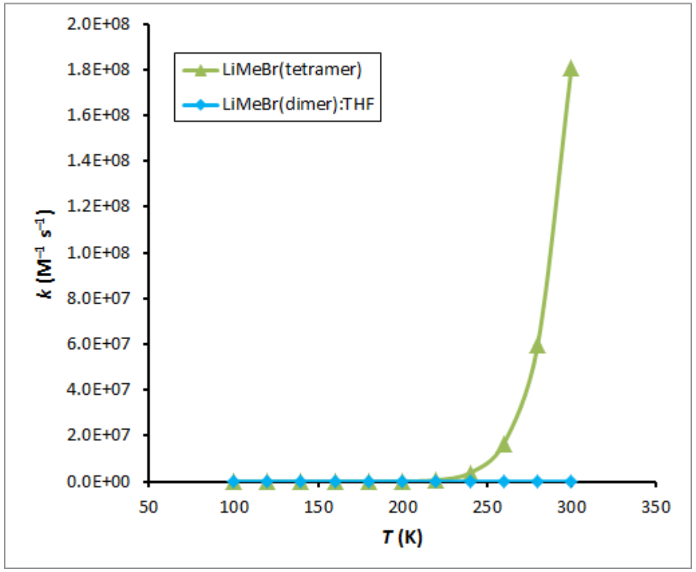


Figure types (design considerations)





- If the context allows, what is graphed and how it is graphed should be determined by some physical law or relationship that underlies the data. <u>Your hypothesis may, in many cases, suggest this relationship</u>.
- In the example on the top left, we are guided by the Arrhenius equation:

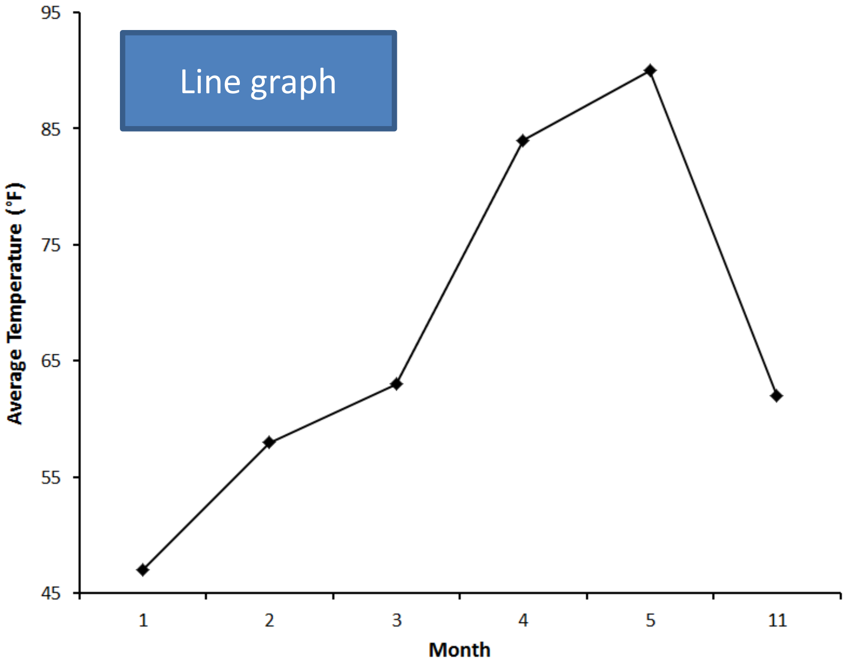
$$k = A \exp[-E_a/RT]$$

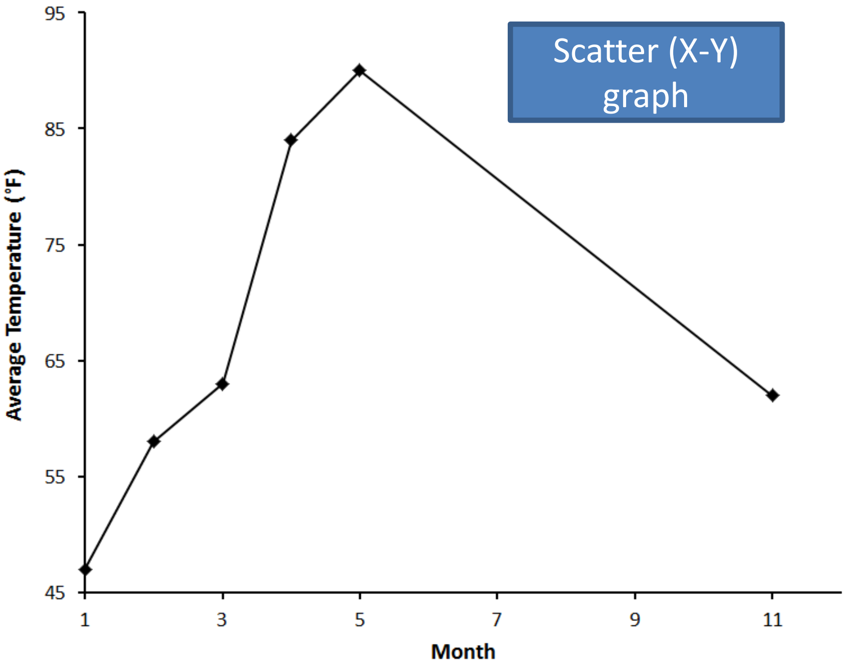
$$\ln(k) = \ln A - E_a/RT$$

- So, ln(k) or log(k) plotted against $1/T$ should yield a straight line, and its slope is $-E_a/R$, i.e., proportional to the activation energy.
- Therefore, the graph on the top left allows us to easily identify the trends in the activation energies in these reactions.
- Plotting some of the same data in another format (as in bottom left) conveys no useful information at all.

Design considerations - continued

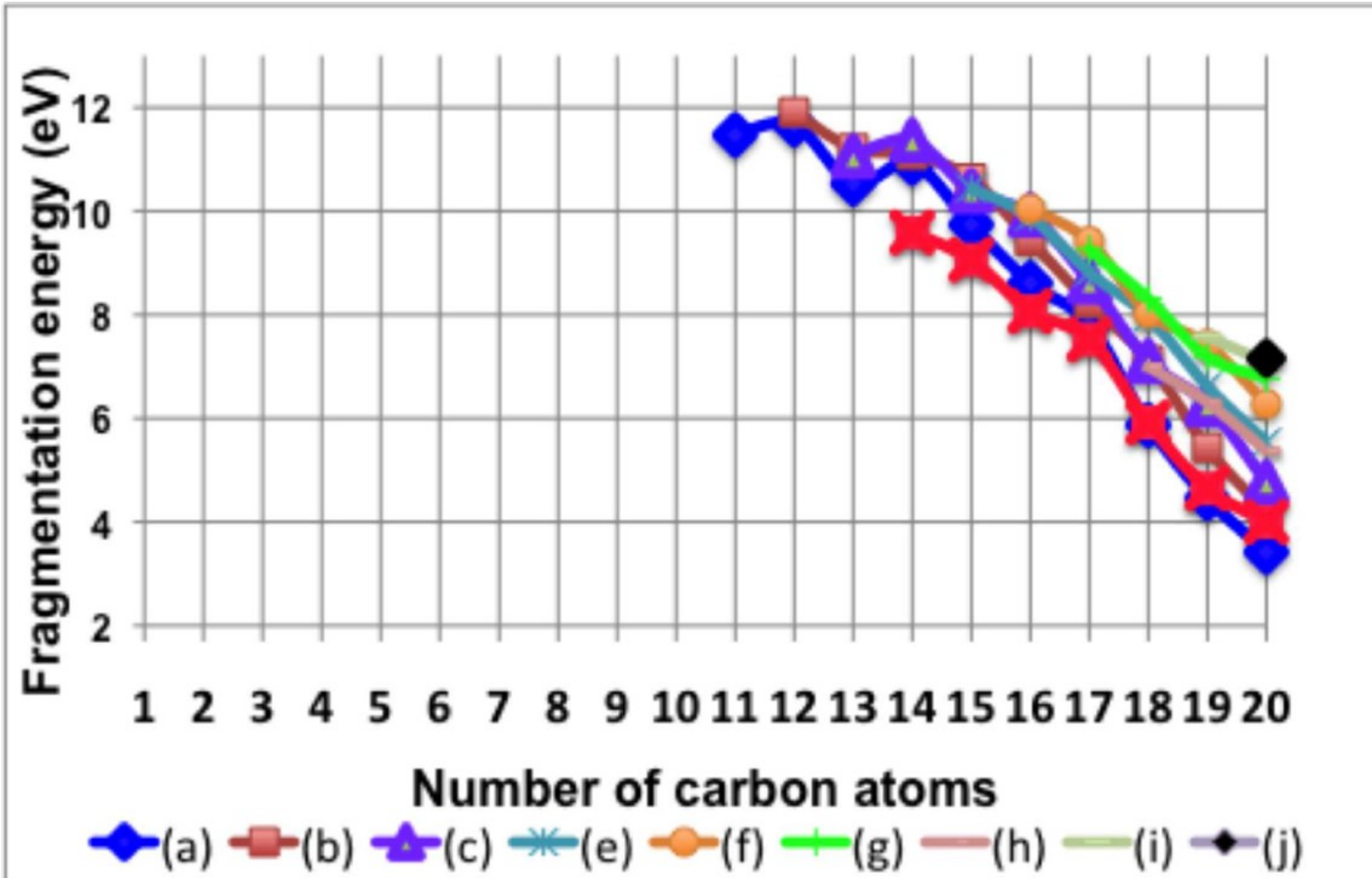
- DO NOT use "line graph" when plotting data that have both X and Y numerical values – in such cases, always use "Scatter" (which is a rather weird name Microsoft has chosen for "X-Y") graph.
- Here is a very artificial (and not entirely appropriate) example.



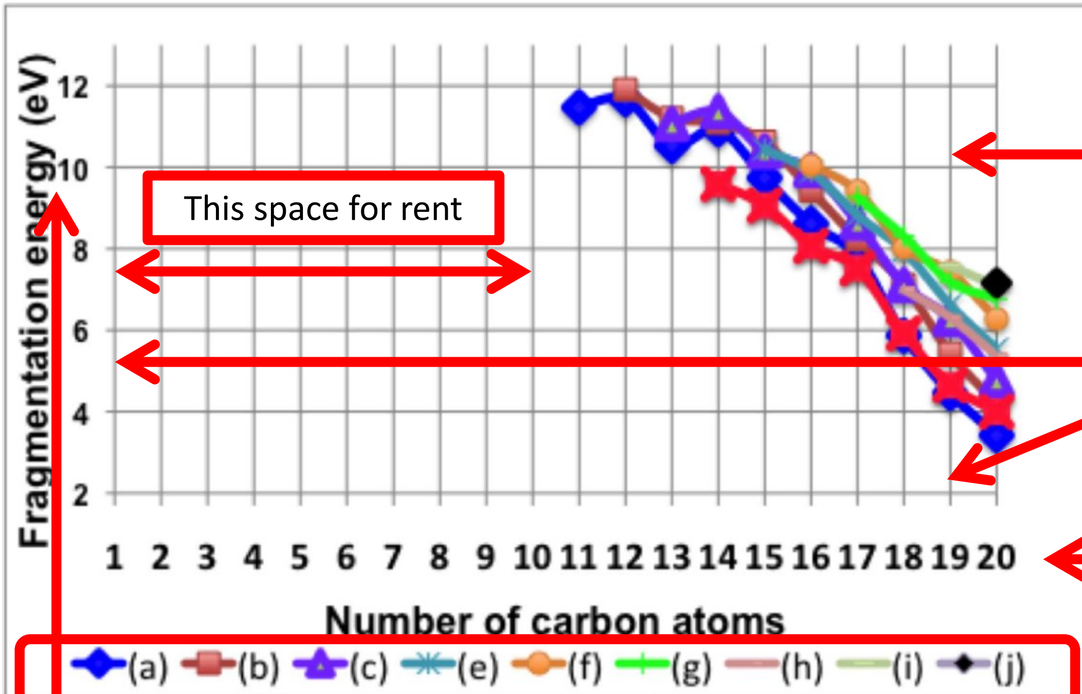


On the left, we use "Line" graph and on the right "Scatter." Note how the appearance of the same data changes.

How many “problems” can you identify?



How many “problems” can you identify?



This space for rent

Eliminate grid lines

Need black line for the axes and tick marks.

Numbering (Rule of 2, 5, 10, …)

Could use some more space (opinion)

Missing line(s); missing letters.
Does the bright red line correspond to (d)?

We should finish off with an excellent figure caption that says nothing useful:

Fig. xx. Results of measurements.

Seeing a figure published is no guarantee that the authors have followed best practices.

Sometimes bad formatting gets past even the editorial staff.

M. V. Reddy, G. V. Subba Rao, and B. V. R. Chowdari, "Metal Oxides and Oxysalts as Anode Materials for Li Ion Batteries," Chemical Reviews, 113(7), 5364-5457 (2013)
DOI: http://dx.doi.org/10.1021/cr3001884

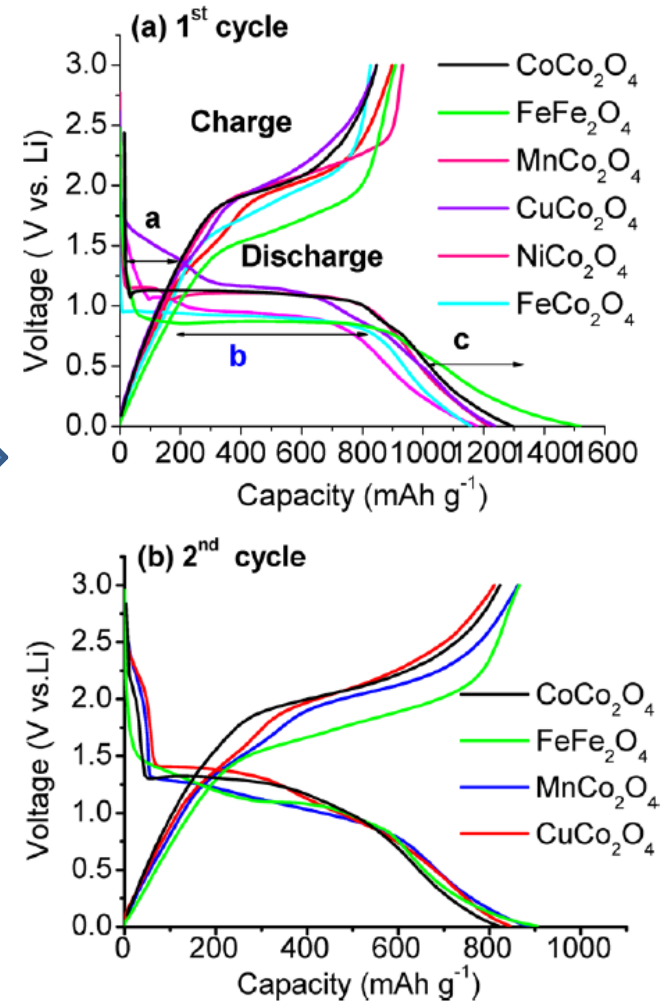
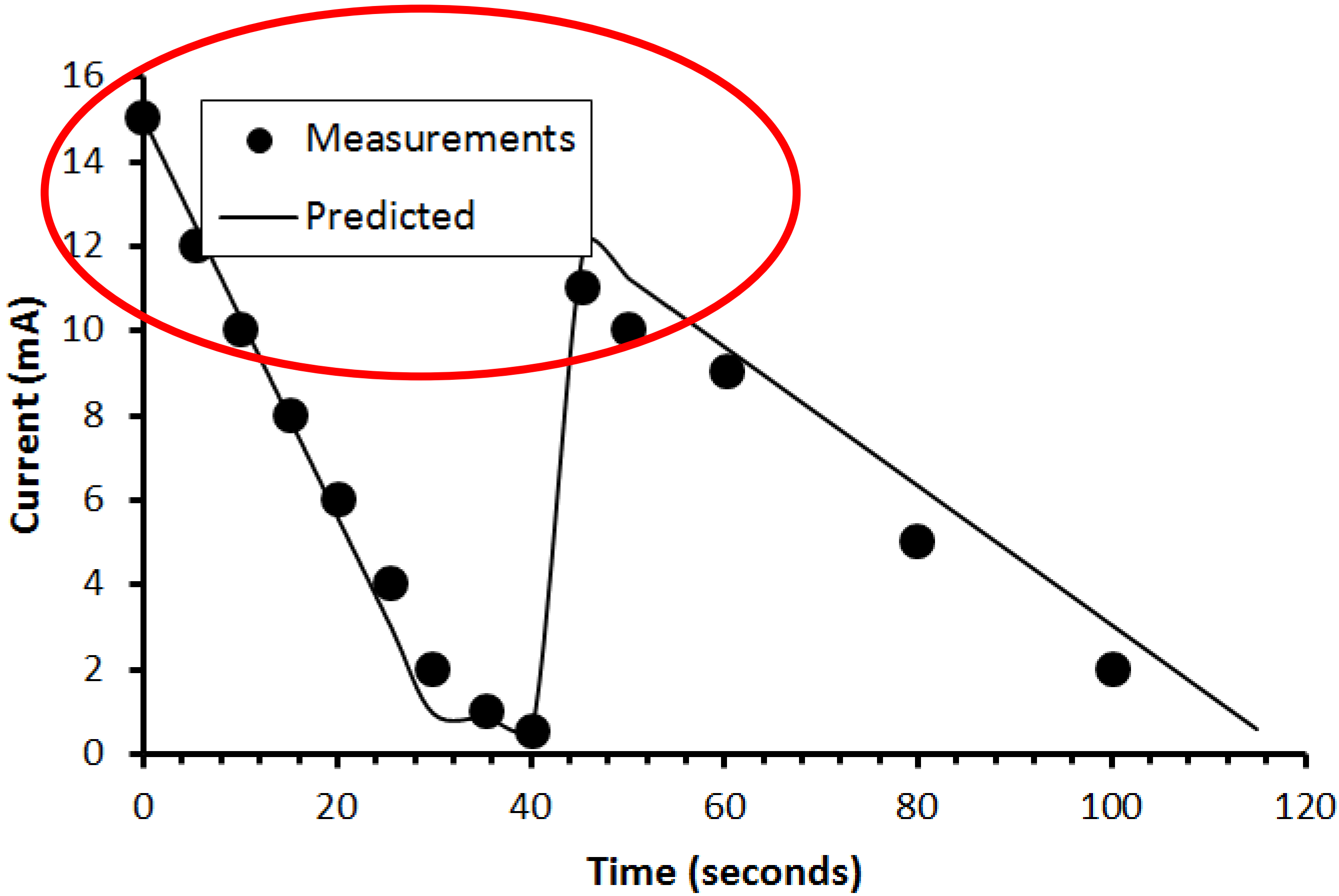
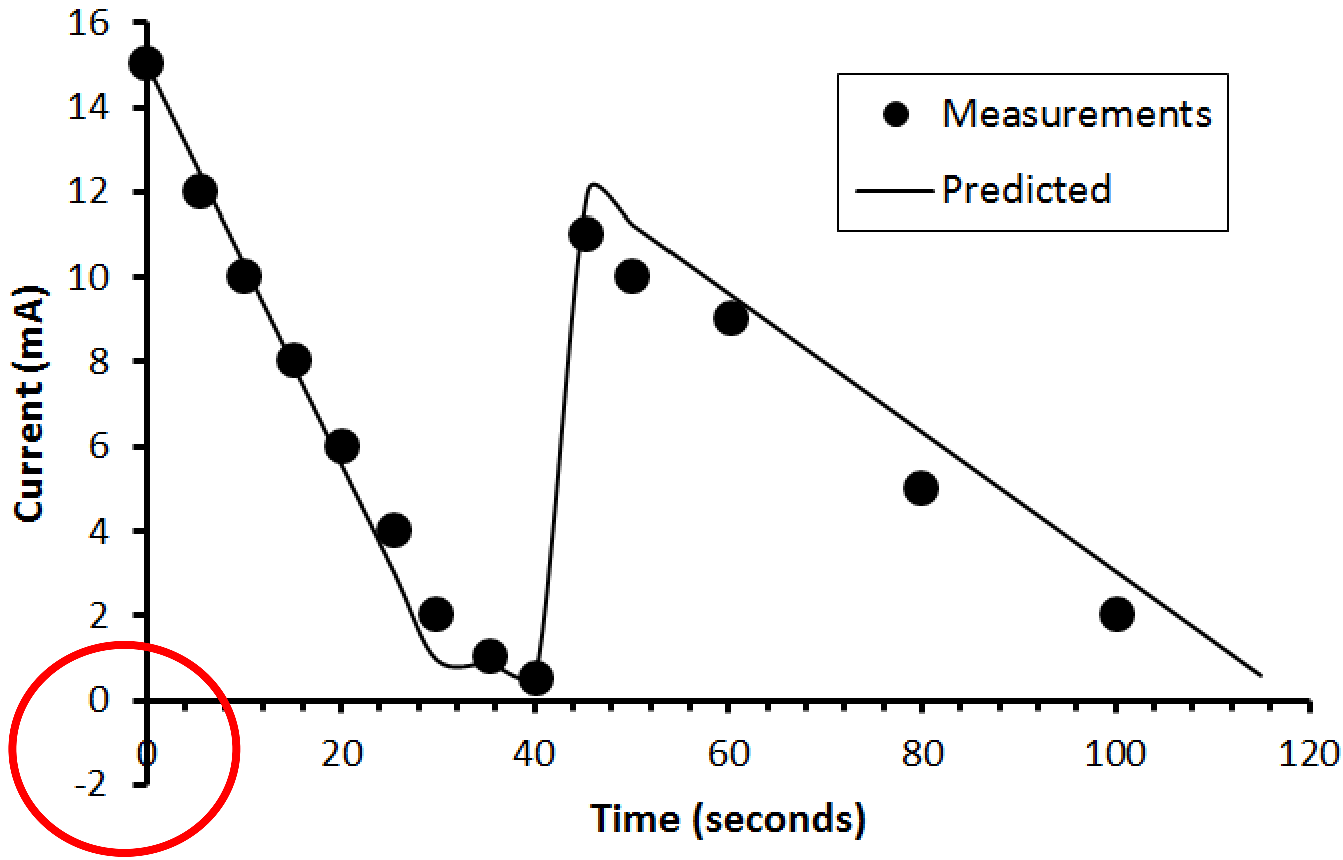


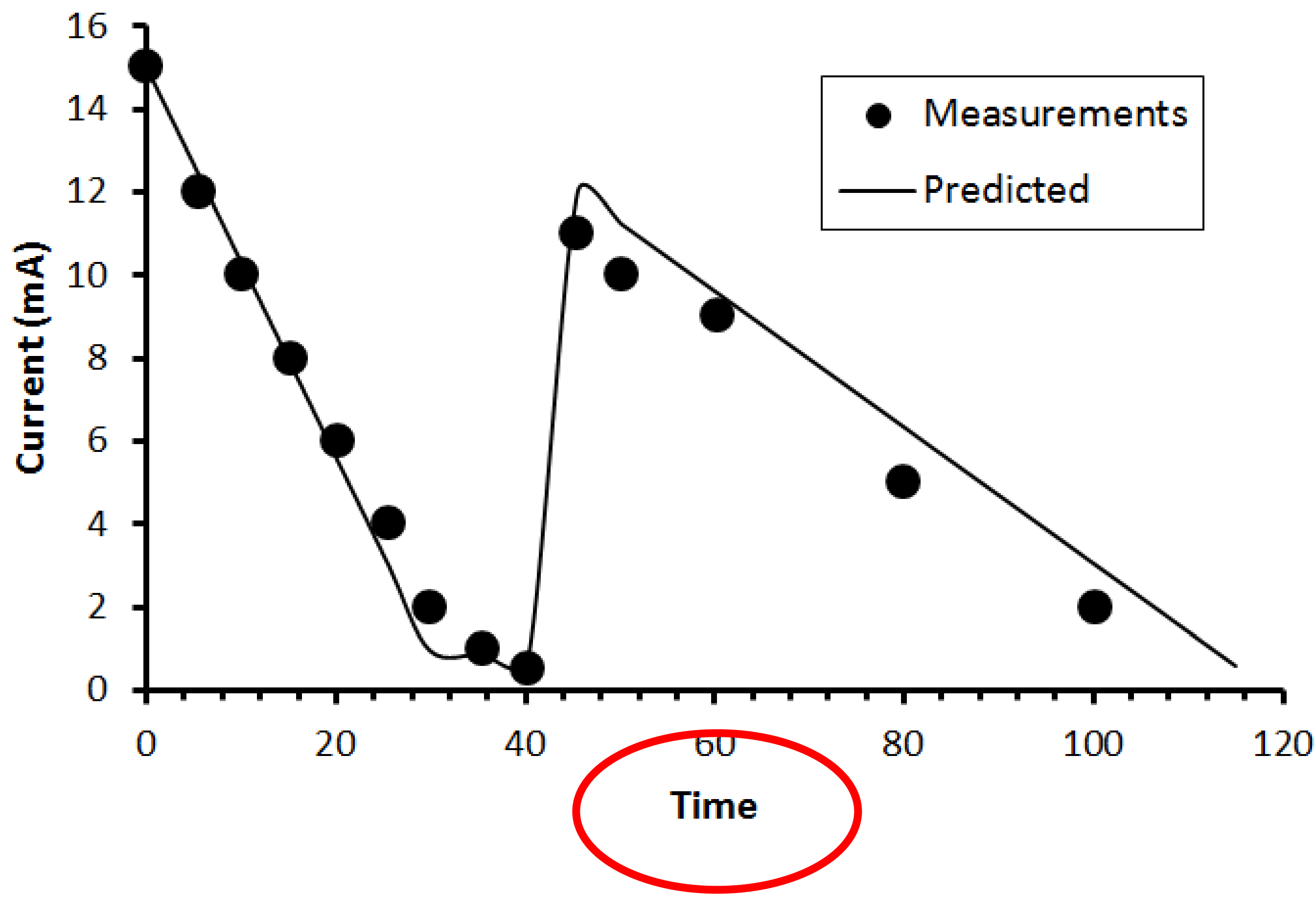
Figure 44. Galvanostatic discharge−charge cycling curves of AB_2O_4 (MM'_2O_4) (A = Co, Fe, Cu, Ni, or Mn, B = Co or Fe). (a) First cycle and (b) second cycle cycled in the voltage range 0.005−3.0 V at current 60 mA g^{-1}. ACo_2O_4 A = Co, Cu, Mn prepared by molten salt method at 280 °C; particle size is on the order of submicrometer; A = Ni or Fe (urea combustion method) and Fe_3O_4 carbothermal reduction method. For comparison, binary spinel (Co_3O_4 and Fe_3O_4) discharge−charge cycling curves are also shown.

Critiques of a few graphs



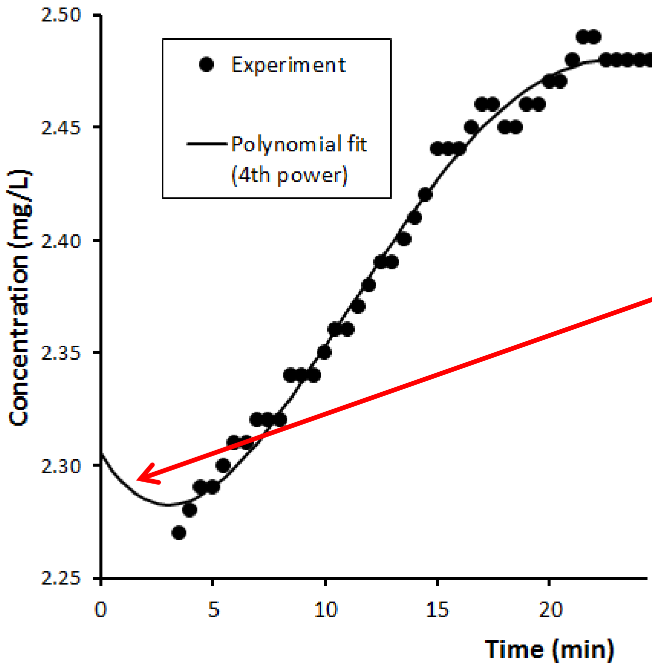
Measurements
Predicted
Current (mA)
Time (seconds)
0
2
4
6
8
10
12
14
16
0
20
40
60
80
100
120


16
14
12
10
8
6
4
2
0
-2
Current (mA)
0
20
40
60
80
100
120
Time (seconds)
Measurements
Predicted


16
14
12
10
8
6
4
2
0
Current (mA)
0
20
40
60
80
100
120
Time
Measurements
Predicted

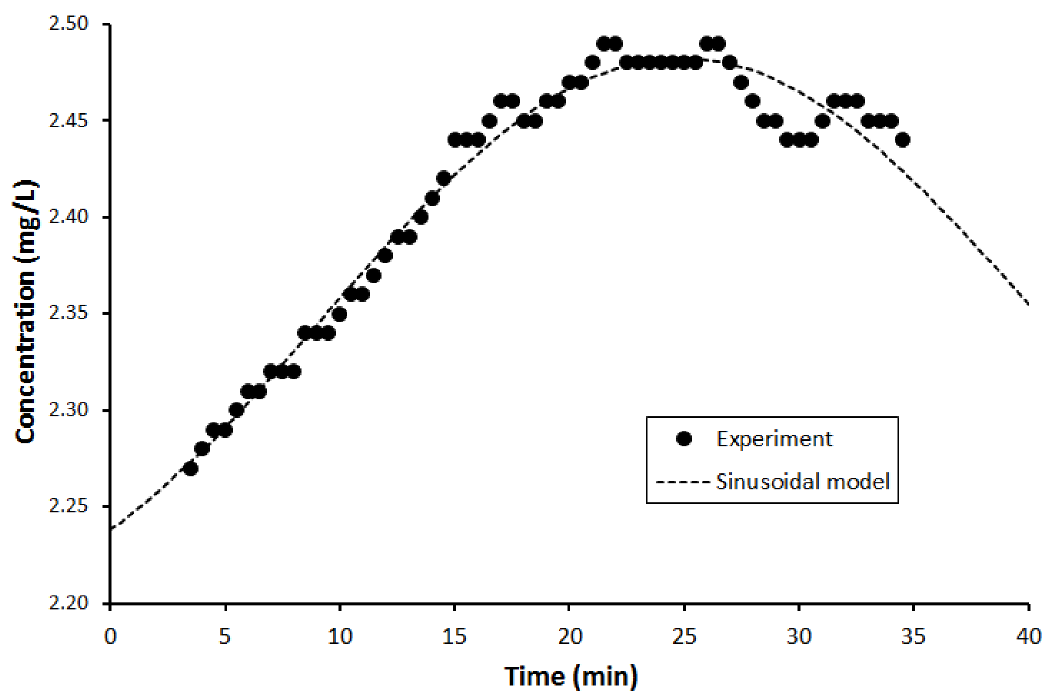
Mathematical models must be based on physical considerations.

Data: Drug concentration in the blood stream after intramuscular administration.

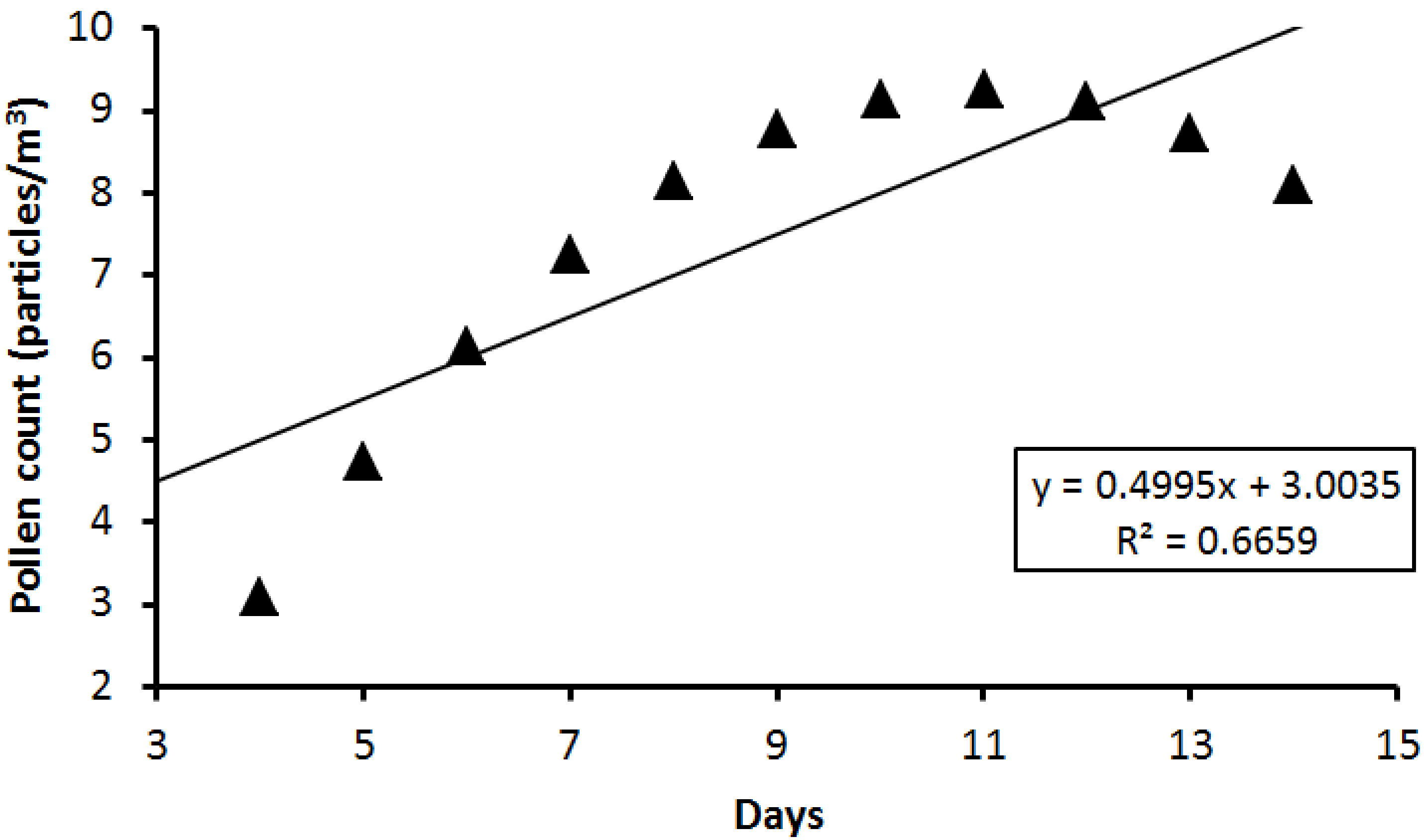


$$f(x) = ax^4 + bx^3 + cx^2 + dx + e$$

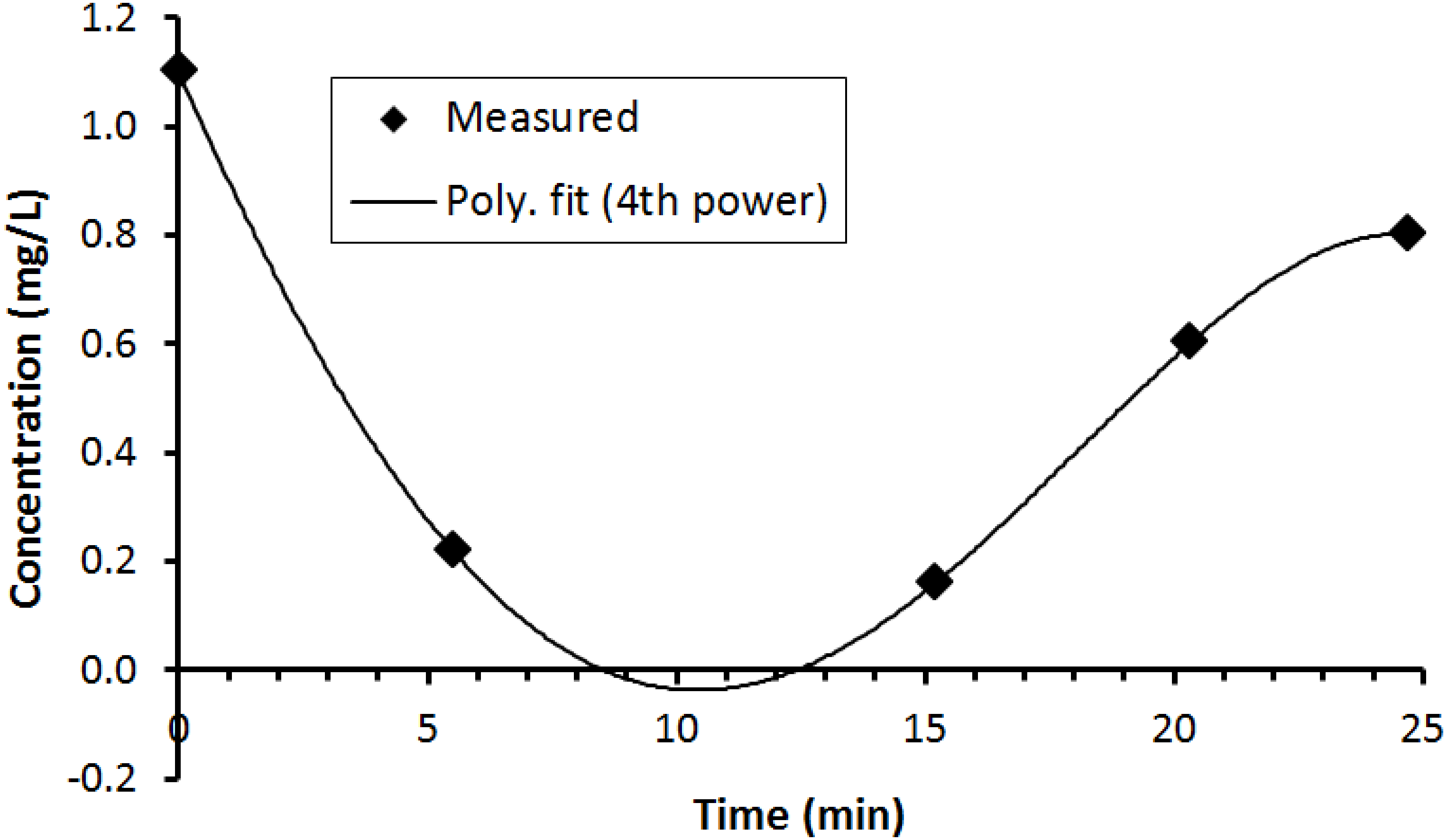
Rise NOT suggested by data!



$$f(x) = a + b\cos(cx + d)$$



Is there a physical justification for the linear fit?



Negative concentrations?

Tables

Presentations should have very few (if any) tables.

Most of the comments to follow apply to tables in papers for publications.

Tables

Table 10. Reaction barriers $\Delta G^{\ddagger}$ (kcal/mol) for the methylene transfer (direct) and carbolithiation (stepwise) pathways of halomethyllithium tetramers and tetramers in the gas phase [Eqs. (13)-(14)] at 173.15 K.

	$\Delta G^{\ddagger}{}_{,B3LYP}$	$\Delta G^{\ddagger}{}_{,MP2}$	$\Delta G^{\ddagger}{}_{,MP2//B3LYP}$
$H_2C{=}CH_2 + (Li\text{-}CH_2\text{-}X)_4 \rightarrow$ TS **12** (concerted)			
X = F	8.07	7.11	7.24
X = Cl	14.74	16.57	16.89
X = Br	8.82	8.14	8.32
$H_2C{=}CH_2 + (Li\text{-}CH_2\text{-}X)_4 \rightarrow$ TS **13** (stepwise)			
X = F	36.23	37.06	37.23
X = Cl	34.26	35.47	35.77
X = Br	32.82	32.24	32.25

- Be a minimalist (fewer lines are better).
- Number the table, give it a sensible caption (the caption should prepare the reader to absorb what is in the table).
- Column headings should make sense (not just to you). Units should be provided either in the heading or as part of the table caption.
- Align the numbers. Decimal numbers should be aligned on the decimal point, NOT centerd!
- If a table has too many columns or too many rows, a different way of presenting the data should be considered.

Tables

Table 10. Reaction barriers $\Delta G^{\ddagger}$ (kcal/mol) for the methylene transfer (direct) and carbolithiation (stepwise) pathways of halomethyllithium tetramers and tetramers in the gas phase [Eqs. (13)-(14)] at 173.15 K.

	$\Delta G^{\ddagger}{}_{,\mathrm{B3LYP}}$	$\Delta G^{\ddagger}{}_{,\mathrm{MP2}}$	$\Delta G^{\ddagger}{}_{,\mathrm{MP2//B3LYP}}$
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X = Cl	34.26	35.47	35.77
X = Br	32.82	32.24	32.25

Note the differences:

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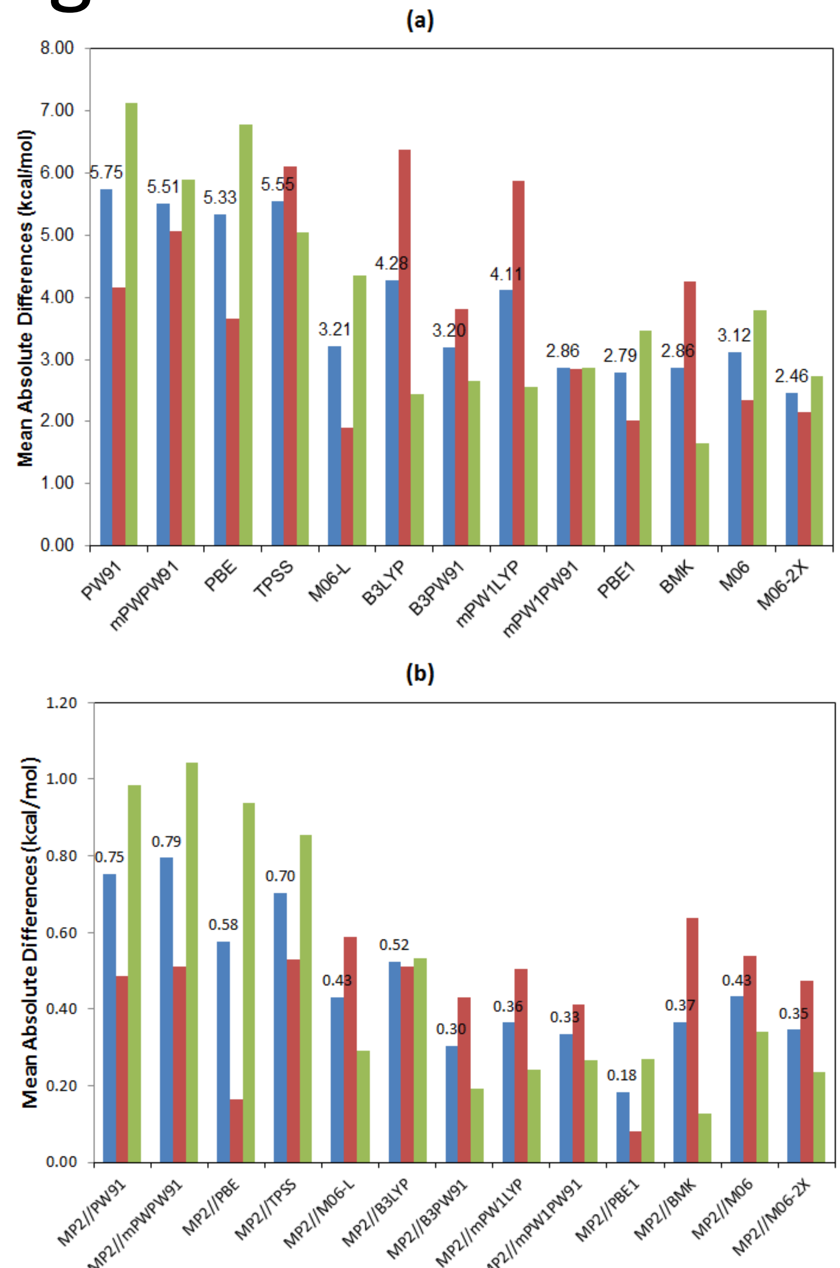
Table vs. figure

Table 8. Mean absolute differences from MP2/6-31+G(d) results for the dataset. The means for the entire dataset, reaction energies (ΔE) only, and reaction barrier heights ($\Delta E^{\ddagger}$) only, are presented.

Method	All	ΔE	$\Delta E^{\ddagger}$
PW91	5.75	4.16	7.13
mPWPW91	5.51	5.07	5.89
PBE	5.33	3.67	6.79
TPSS	5.55	6.11	5.05
M06-L	3.21	1.91	4.36
B3LYP	4.28	6.38	2.45
B3PW91	3.20	3.82	2.65
mPW1LYP	4.11	5.88	2.56
mPW1PW91	2.86	2.86	2.87
PBE1	2.79	2.01	3.47
BMK	2.86	4.25	1.65
M06	3.12	2.34	3.80
M06-2X	2.46	2.15	2.73
MP2//PW91	0.75	0.49	0.98
MP2//mPWPW91	0.79	0.51	1.04
MP2//PBE	0.58	0.17	0.94
MP2//TPSS	0.70	0.53	0.85
MP2//M06-L	0.43	0.59	0.29
MP2//B3LYP	0.52	0.51	0.53
MP2//B3PW91	0.30	0.43	0.19
MP2//mPW1LYP	0.36	0.50	0.24
MP2//mPW1PW91	0.33	0.41	0.27
MP2//PBE1	0.18	0.08	0.27
MP2//BMK	0.37	0.64	0.13
MP2//M06	0.43	0.54	0.34
MP2//M06-2X	0.35	0.47	0.23



We are visual creatures. Most of the time, a figure gets the message across more efficiently.

Table vs. figure

There were three reasons to split the figure into (a) and (b) (at the green line below):

1. Incorporating all these bars into a single figure would have made it a lo…ng figure OR a very cluttered one.
2. The bars in (b) are much shorter. Putting them into (a) would have made them look like grass growing under trees, and reduced the value of the graphical representation.
3. There is a logical place to split the data into two panels.

M06	3.12	2.34	3.80
M06-2X	2.46	2.15	2.73
MP2//PW91	0.75	0.49	0.98
MP2//mPWPW91	0.79	0.51	1.04
MP2//PBE	0.58	0.17	0.94
MP2//TPSS	0.70	0.53	0.85
MP2//M06-L	0.43	0.59	0.29
MP2//B3LYP	0.52	0.51	0.53
MP2//B3PW91	0.30	0.43	0.19
MP2//mPW1LYP	0.36	0.50	0.24
MP2//mPW1PW91	0.33	0.41	0.27
MP2//PBE1	0.18	0.08	0.27
MP2//BMK	0.37	0.64	0.13
MP2//M06	0.43	0.54	0.34
MP2//M06-2X	0.35	0.47	0.23