The Journal of Physical Chemistry Letters

Editorial

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Graphical Excellence

It is the experience of every author that figures and illustrations in scientific papers are the gateway for effective communication of research findings to the scientific world. While the title and abstract of the paper draw the attention of any avid reader, the essence of the paper is captured by the figures and schemes. Well-drawn, scientifically correct figures make the first impression of the scientific findings. Yet, time and time again, we see poorly presented results, inaccuracy in plotted data, improperly defined axes, meaningless significant digits in axis scales, wrong or missing units, and undefined symbols or traces. Such inaccuracies can lead to *reject recommendations* from the editors and reviewers. We wonder *why researchers who are passionate about communicating their findings, many times take little interest in effective presentation of their data.*

The ease of computer software usage has contributed to some of the inattentiveness for presentation of data. Not too long ago, researchers plotted data on a graph sheet with a pencil. The origin was inserted first as (0, 0) and not with decimals, (e.g., (0.00, 0.00)) as you commonly see in many of the software-produced plots. (*Note: Absolute zero has no decimals, but it is difficult to override the format in most plotting software.*) The researchers would then decide on the choice of scale, major ticks, units, and so forth. They inserted data points and checked the validity of any analytical solution included in the study. Straight line plots were explained with a supporting expression (e.g., kinetic plots). The manual checks at each step ensured accuracy of the data presentation. It was not a common practice to connect points on a plot; instead, a *French curve* or *flexible curve* was used to draw a trend line. Today, you select the data in a spreadsheet and let the computer figure out the plot. (Otherwise, how can you explain four or more significant digits for subnanosecond lifetimes and associated rate constants when the excitation pulse has a pulse width of few nanoseconds or plots with no relationship between the *X*- and *Y*-axis as in relating an observed property with sample numbers or solvent names?)

The above discrepancies are not meant to imply that modern platforms of computer software are error-ridden. It is carelessness on the part of the researcher that contributes to the misrepresentation of the data. Analytical software programs are great tools for analyzing complex sets of data, and their contribution to modern science is undeniably important and significant. However, it is important to know the data collection procedure, limitations of the measurements, and the variation (error bars) in the distribution of values while processing the data with any available software. Figures that are produced with care and accuracy help to demonstrate the quality and reliability of research.

There are two aspects that need to be considered while drawing figures: (1) accuracy of data presentation and (2) aesthetics of the figure. According to Tufte, a figure or graphic is a well-designed presentation of interesting data that consists of complex ideas communicated with **clarity** (no ambiguity or confusion), **precision** (truthful results with no distortions), and **efficiency** (minimal "chart junk").[1] *It gives the viewer the greatest number of ideas in the shortest time with the least ink in the smallest space.* A well-composed graphic art with a complete description should stand alone, and the reader should be able to grasp the essence of the experiment as well as the analysis of the result.

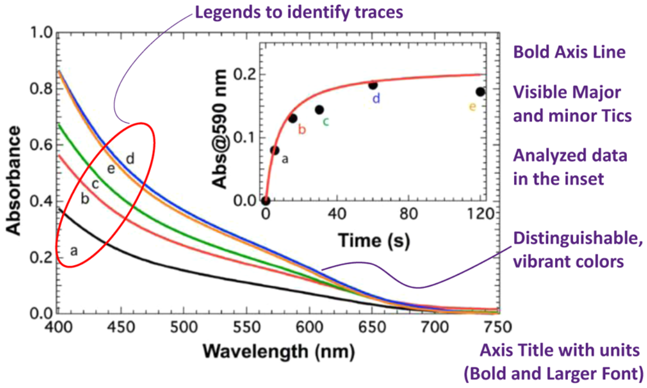

Figure 1. An example of graphical presentation of data. A few items in the figure are highlighted for clarity and accuracy of the presentation. Reproduced from ref 4.

We will now discuss important instructions that the authors can follow while preparing graphics for a scientific figure. A number of useful tips are summarized in Table 1, and we also note the examples given in Figure 1, which was taken from an earlier published paper. Although the focus of this Editorial is intended for preparing physical chemistry papers, readers from other disciplines can also find these tips useful.

Improving the Effectiveness of Data Presentation. Since ACS journals do not charge to reproduce colored figures, authors should make use of this feature to enhance the effectiveness of their figures. It is important to select colors that distinguish each data set and to use vibrant and bold colors in an appealing way. The choice of symbols and traces should be made wisely to represent multiple data sets. Avoid using curves with the same colors that are distinguished by dashes and dots as they lack distinguishability for closely spaced curves. It is also important to take into consideration the size of the figure. The "golden rectangle" (height/width, 1:1.6) is an appealing size for figures. Combining a set of related figures into a single panel is also an effective way to present multiple set of results related to the same experiment.

Selecting Proper Axis and Units. Once the data have been collected and analyzed, the author should decide the best possible way to present the results so that the reader can visualize the theme and conclusions of the experiment. Decide whether an *X*−*Y* plot or bar diagram is appropriate for presenting the data. For an *X*−*Y* plot, there should be a direct causality or relationship. For example, sample names/numbers or different solvents if presented on the *X*-axis do not bring in causality. However, a sample or solvent property can show an important relationship with the *Y*-axis. *Comparative data with no direct relationship between the X- and Y-axes should be presented as a bar diagram.*

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Table 1. Tips for Drawing Effective Scientific Figures

	Common problems/ misrepresentations	Suggestions for correct format/presentation
Axis scale	unreadable text	Try to maintain the text font size of 18 or greater in the original drawing.
	axis crowded with text and numbers	Use major and minor ticks, and limit the number of entries on the scale (no more than five entries).
	unnecessary significant digits (e.g., 400.000 nm for a wavelength scale)	Know the accuracy of the data measurement when determining significant digits.
	symbols in the text (ex: λ (nm))	Avoid symbols because they may have different definitions within the same field (e.g., λ as a symbol for wavelength and reorganization energy). For special cases when symbols are used as axis titles, they need to be defined in the caption (e.g., define k_{et} in the title as a rate constant of the electron or energy transfer).
	missing scale on the *Y*-axis	The *Y*-axis scale (or scale bar) should be included for providing quantitative information. For example, having an absorbance scale lets the readers know the absorptivity of the sample.
Scientific units	missing units on the scale	When appropriate, the axis title should be accompanied by units (preferably SI unit nomenclature). Ratios, fractions, or logarithmic numbers should not carry any units. Pay special attention to prefixes such as m (milli), μ (micro), n (nano), p (pico), etc.
	Fraction or percentage?	Make sure the representation is accurate and explain the terms in the caption. For composition ratios, indicate wt/wt or vol/vol in the caption.
	dimensionless units or inclusion of units	Both wavelength/nm or wavelength (nm) are acceptable formats. The same format, however, should be used for all figures within the manuscript.
	arbitrary/relative/normalized scale	Know the difference between these prefixes. They are not interchangeable. Explain the context in the caption.
	defining absorbance with units (au)	Absorbance is the logarithm of a ratio of intensities and hence does not have any units. (The same is true for pH.) Absorbance should be represented by the numbers as recorded from the spectrophotometer. Do not refer to absorbance with au. An absorbance spectrum presented without scale does not bring credibility to the data.
Plotting data	*X*−*Y* plot versus bar diagram	Causality between *X*−*Y* axes (direct relationship between *X*- and *Y*-variables) is needed. If there is no relationship (e.g., a catalytic property representing different samples or an *X*-axis showing different solvents), the data should be presented as a bar diagram. The axis should be defined with a property and not the name of the sample for *X*−*Y* plots.
	complex 2-D and 3-D plots	Color plots are great for visual displays. Presentation of these plots should convey the science associated with the data clearly and convincingly. Make sure the general readership is able to comprehend the complexity of the presented data.
	error bars	Include error bars in the data points, and indicate in the caption the type of error (standard deviation, standard error, etc.) and whether the error bars represent multiple measurements on the same sample or different samples. Describe the method of analysis in the caption.
	trend line	Know the difference between connecting the data points and drawing a smooth trend line. Make sure there are more than five points when showing a trend in the experimental results. If the line is only meant to be a guide-to-the eye, indicate this in the caption.
	unreadable scale bars in electron micrographs	Make sure there is a readable scale bar in every micrograph. If necessary, include the scale bar dimensions in the figure caption.
	computer screen dump as part of the figure	While it is easy to copy and paste a screen dump, the figures are often blurred or the fonts not readable. Every modern instrument has the capability to export data files, and the researchers should make use of it.
Data highlights	choice of colors	Use bold and vibrant colors (black, blue, red, green) that distinctly show differences between the data points/traces.
	identifying traces with color names	Avoid identifying traces with color names in the caption. Color-blind researchers have difficulty in associating colors in the text with those in traces. Each trace should be identified with a legend (*a,b,c etc.*) so that when the graphic is reproduced on a B&W printer, they can be identified properly.
Figure caption	missing details	The caption is an important part of the figure and should provide all of the details (e.g., concentrations, medium, temperature, and other experimental conditions) Add a description of the analysis, if applicable.
	identifying individual traces or data sets	It is important that each trace is properly identified so that the reader can quickly capture the difference between data sets. Explain the analysis used to fit the data.
	reproduced data	If figures are reproduced from another paper, it should be properly credited in the caption and proper permissions should be obtained.

Mark the scale with major and minor ticks, and insert appropriate units. Use appropriate axes titles with scientifically acceptable units in bold letters. Logarithmic expressions used to derive the measured value (e.g., absorbance, pH, etc.) do not have any units. *Do not present absorbance with* ***au*** *as can be seen in many recent publications.* Use the same format of font size, color coordination, and representation in all of the figures in the paper. The text within the plots and insets should also be clearly readable, with the minimum font size no smaller than half that of the main text in the paper.

Error Bars. When presenting data, it is very important to communicate the accuracy of the measurements to the reader. Thus, tables of measurements should have error estimates, and figures should have error bars. When plotting primary data, such as spectra, transient absorption traces, cyclic voltammetry measurements, or temperature-programmed desorption data, it is acceptable to leave out the error bars (the errors associated with this type of data are usually small). However, error bars must be included for figures that present data derived from the primary measurements.

There are a variety of different ways of reporting errors, and the appropriate method depends on the data being presented. For example, in nanoparticle research, for plots of data versus particle size, it is common to use the standard deviation of the size as an error estimate (this gives the reader an idea about the range of sizes that contribute to the measurements). For data that represent an average of different measurements, the standard error (the standard deviation of the data divided by $\sqrt{N}$, where N is the number of measurements) or the 95% confidence limit (roughly 2× the standard error) should be used.[2] When the data being plotted are obtained from fitting experimental measurements, the standard error derived by the fitting program can be used. The type of error being used should be given in the figure caption. In some cases, the errors are very small, so that they are smaller than the size of the symbols used in the figure. In this case, a statement to this effect should be included in the figure caption.

Sometimes, the errors generated from fitting programs can seem unreasonably large or unreasonably small. If it does not look right, then you can vary the parameters in the fitting function and see for yourself how this changes the fit. This type of sensitivity analysis can be time-consuming, but it yields the range of values that gives a reasonable fit to the data. Finally, the quantity being plotted is often the result of several different types of measurements, each of which has an error associated with them. For this type of data, the usual rules of error propagation have to be used to determine the total error.[2] Often, it seems that it is harder to determine the error than the actual value of the quantity being reported, but the effort is worthwhile; proper error analysis gives the reader confidence that the data being reported are reliable.

Figure Captions. The description of the figure is intended to explain the data and analysis so that the reader can fully appreciate the scientific value of the results. Proper identification of the data sets and analysis is an integral part of the caption. Every effort should be made to include experimental or analytical details so that the reader gets complete understanding of the data being presented. Any data reproduced from another paper should be properly identified and credited. While preparing a manuscript for submission to *JPCL*, please remember to include the figure caption below the figure so that it is easily read by editors and reviewers (and embed all figures and captions within the text).

Schemes and Illustrations. Schemes and illustrations are usually conceptual ideas that assist authors to explain their scientific findings. Often, the schemes are an effective tool to steer the readers into an imaginative scientific concept. TOC graphics have also become an integral part of the paper.[3] Avoid being excessive in drawing schemes and illustrations beyond the scientific representation. Authors should avoid the use of cartoons and smiley faces in their TOC graphics as they undermine their scientific credibility. Such TOC graphics are not accepted in *JPCL* or other *JPC* journals.

For greater impact of published papers, we suggest that the total number of figures and schemes in a manuscript be kept to a minimum. The figures included in the main text should present key results that serve as the basis of scientific discussion. Additional supporting data, such as sample characterization (e.g., absorption and emission spectra, XRD, TEM images, etc.), data analysis, and experimental set up can be included in the Supporting Information. Papers composed for *JPCL* should contain a maximum of five figures/schemes in the main text.

In summary, well-composed and scientifically accurate figures constitute the core of a scientific paper. A little extra care in presentation of the data can increase the impact of published work and draw the attention from the broader scientific community. The readers may also benefit from an earlier Editorial on composing a scientifically effective paper.[4]

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Views expressed in this editorial are those of the authors and not necessarily the views of the ACS.

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REFERENCES

(1) Tufte, E. R. *The Visual Display of Quantitative Information*; Graphics Press: Cheshire, CT, 1983; pp 1−197.

(2) See, for example: Lyons, L. *A Practical Guide to Data Analysis for Physical Science Students*; Cambridge University Press: Cambridge, U.K., 1991.

(3) Buriak, J. M. Titles and Table of Contents Images: The Candy Store Analogy. *Chem. Mater.* **2014**, *26*, 1289−1290, DOI: 10.1021/cm500170v.

(4) Kamat, P.; Schatz, G. C. How to Make Your Next Paper Scientifically Effective. *J. Phys. Chem. Lett.* **2013**, *4*, 1578−1581, DOI: 10.1021/jz4006916.