Automating Spectrophotometic Tirations

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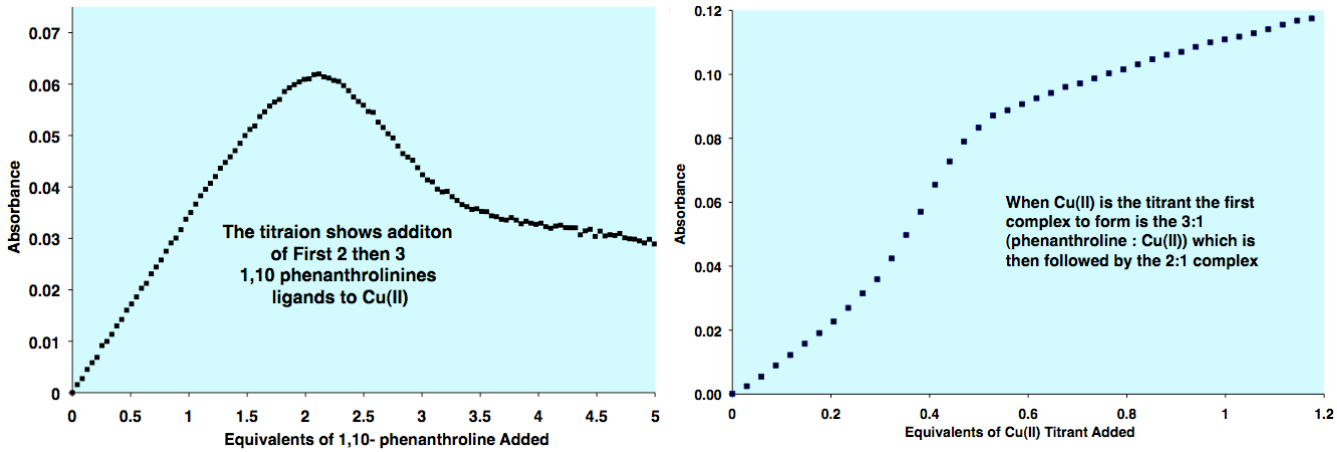
Everyone reading this is no doubt familiar with Beer's law and its use to determine concentration from absorbance. Likewise, you are almost certain to recall joyful hours using titration methods of determining one substance by metering its reaction with another. Spectrophotometric titrations marries the power of these two methods together. Since modern instruments manage the task of experimental control and data acquisition quite handily, it is the details of data analysis that remain to be automated.

Generally, the events of chemistry are documented in before and after photos, but what about the journey? If every picture tells a story, why not record a time-laps progression of a reaction? Why not capture a 3-D record as the story unfolds? Well, just as camcorders capture live action, chemical reactions can be captured. In fact the technology is so powerful a record of all absorbance changes occurring over several hundred nanometers can be taken each 0.25 nanoseconds! The topography of such an information mountain may seem too much to ponder, but like all mountains there are only certain veins worth mining for information.

Below are two pictures of the reaction between Cu^{2+} and 1,10-phenanthroline recorded at 670 nm. On the left, when Cu^{2+} and is in excess, the reaction sequence follows the path of first forming the 2:1 complex, then, reluctantly, forming the 3:1 complex. On the right, when 1,10-phenanthroline is in excess, this reaction sequence is exactly reversed, i.e. first 3:1 then 2:1. Riddling out the details of the events evident in the steps, slopes, and curvatures, exhibited in various reaction views will be the kind of job the student selected for this project will do. Please remember that the pictures displayed below only illustrate the changes occurring at one wavelength. It is quite reasonable to expect the topography manifested at other wavelengths may provide additional helpful details. Earlier work by Ivan Zubkov documented a similar experimental pathway[1].



The student matched with this project will be encouraged to report on the results of their work at a professional meeting; perhaps the Joint Southwest-Southeast Regional Meeting of the American Chemical Society in New Orleans in 2010.

1) "Development of Algorithms for Automated Spectrophotometric Titrations," Ivan P. Zubkov and John A. Lynch, *Microchemical Journal*, 90, 13-18 (2008).