Letters

Using and Adapting the Box-and-Dot Method To Determine Significant Figures

I enjoyed the recent article by Stephenson entitled "The Box-and-Dot Method: A Simple Strategy for Counting Significant Figures" *(1)*, and I am glad that he has shared this clear and simple method. This is essentially the approach I have used in my own lectures for a number of years, with one minor change that may make this more clear for students.

My concern is that there may be some confusion among the students when two distinct boxes result. Therefore, rather than using a box, I simply underline the significant figures. Thus, after all three steps, the students always produce one, continuous line under the appropriate digits. Alternatively, it would be straightforward to apply this method using the overbar convention.

Literature Cited

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Chemical Speciation and Calculation of Sports Drink pH

We wish to comment on the article by Drossman *(1)*, "Chemical Speciation Analysis of Sports Drinks by Acid−Base Titrimetry and Ion Chromatography: A Challenging Beverage Formulation Project", and the subsequent letter by Guiñón-Segura *(2)*. Our comment relates to the calculation of the sample pH. Drossman used a pointer function to find the calculated pH of a sample containing 12.5 mM citrate, 0.239 mM phosphate, 9.82 mM chloride, 9.82 mM sodium, and 3.2 mM potassium. Guiñón-Segura showed how to solve for the pH for the same sample using Mathcad.

We recently became aware of a versatile Excel spreadsheet with embedded macros, *CurTiPot*, which was developed by I. G. R. Gutz of Universidad de São Paulo and is freely available on the Internet *(3)*. *CurTiPot* was originally created to simulate titration curves, but now includes a pH calculator and more *(4, 5)*. The user interface of *CurTiPot* is easily accessible by a general chemistry student with almost no instruction. It incorporates activity coefficients by means of the Davies equation *(6)*. Neither Drossman nor Guiñón-Segura included the effects of activity coefficients in their calculation of pH, although the ionic strength is low in this problem and so inconsequential.

To illustrate the calculation of a sample pH with chemical composition given in the first paragraph, we input the data into *CurTiPot*: 0.239 mM PO_4^{3-}, 0.828 mM Cit^{3-}, and 11.672 mM H_3Cit along with the requisite Cl^-, Na^+, and K^+ concentrations. The calculated pH is 2.83, which is in close agreement with experimental value of 2.85, the Drossman pointer value of 2.85, and the Guiñón-Segura Mathcad value of 2.83.

We summarize some aspects of using *CurTiPot*: (i) The database contains pK_a values for about 250 common aqueous acids, including citric acid and phosphoric acid, and the user can easily introduce an acid that is not in the database. (ii) The equilibrium concentrations of all species in solution are part of the output and these values compare well to the values of the previous authors. (iii) The computational algorithm is robust. (iv) We have developed a question related to this problem that could be used as homework or on an examination and it is included in the supporting information.

Literature Cited

1. Drossman, H. *J. Chem. Educ.* **2007**, *84*, 124–127.
2. Guiñón-Segura, J. L. *J. Chem. Educ.* **2008**, *85*, 371.
3. pH Calculations and Acid−Base Titration Curves. http://www2.iq.usp.br/docente/gutz/Curtipot_.html (accessed May 2010).
4. Fornaro, A.; Gutz, I. G. R. *Atmos. Environ.* **2006**, *40*, 5880–5892.
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6. Davies, C. W. *Ion Association*; Butterworths: London, 1962, pp 37−53.

Supporting Information Available

A homework problem using *CurTiPot* to calculate the pH of a sports drink. This material is available via the Internet at http://pubs.acs.org.

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