11.4: The Use of Models in Introductory Chemistry

The *Journal of Chemical Education* has published three responses (*1*,*2*,*3*) to a paper Roger DeKock and I published stressing the importance of kinetic energy in interpreting trends in atomic ionization energies (*4*). We have previously responded to Carlton (*5*, *6*), and I would now like to respond to Gillespie, Moog, and Spencer. We have jointly submitted a response to John P. Lowe, a copy of which can be found on this page.

For the most part Gillespie, Moog, and Spencer (*1*) defend themselves against criticisms we do not make and ignore the major argument we do make. For example, we do not criticize the use of the shell model to teach the most basic elements of atomic structure in introductory chemistry courses. However, we do challenge the use of the shell model for purposes that extend beyond its range of validity.

Among these would be the use of the shell model to explain the trend of ionization energies within a given shell and the more fundamental issue of atomic stability. With regard to the former, one asks why is the ionization energy for He less than twice that for H? With regard to the latter, one asks why doesn't the electron collapse into the nucleus under the electrostatic force of attraction between the electron and the nucleus? The shell model has much to offer as a pedagogical tool to answer some rudimentary questions about atomic and molecular structure, but it cannot answer these question. Quantum mechanics is required to answer questions of this type as we demonstrated in our critique.

Gillespie, Moog, and Spencer concede that our criticism is valid within the context of quantum mechanics, implying that quantum mechanics is just another model on the menu of models that could be used to explain atomic and molecular phenomena. For example, they say,

At the general chemistry level it is probably sufficient to state simply that the high IE of He with respect to H is due to the greater attraction of the nucleus for electrons, offset by the repulsion between electrons.

Unfortunately this is not a valid explanation as we demonstrated in our critique. In attempting to reach and educate all of the constituencies of general chemistry, we should not over-simplify the concepts because it makes them easier to teach. Teaching simple models that students can easily digest is tempting, but these easily digestible models are frequently fundamentally incorrect. Perhaps these incorrect models do no great harm at the introductory level simply because general chemistry is a terminal course for most of those who take it, and the retention half-life for the good or the bad content is relatively short. However, over-simplifications must eventually must be un-taught, or retracted, at some later time in the education of the chemistry major or others who study chemistry beyond the general chemistry sequence. The explanation by Gillespie *et al.* for the H/He ionization ratio falls into this category. It has to be retracted eventually, so why teach it at all?

Why not simply state that the answer to the question of the trend in ionization energies within the shells (or the explanation of atomic stability) is too complicated for general chemistry students. Valid explanations require quantum mechanics which, for chemistry majors, will be encountered in the junior or senior year. Furthermore, quantum mechanics is not just another mouse click on the model menu, it is the benchmark theory, the one against which all other approximate models are judged. For example, in their seminal treatise on molecular mechanics Burkert and Allinger wrote (*8*),

Calculations that do not use the Schrödinger equation are acceptable only to the extent that they reproduce the results of high level quantum mechanical calculations.

Literature cited:

1. Gillespie, R. J.; Moog, R. S.; Spencer, J. N. *J. Chem. Educ*. **1998**, *75*, 539-540.
2. Carlton, T. S. *J. Chem. Educ*. **1999**, *76*, 605.
3. Lowe, J. P. *J. Chem. Educ*. **2000**, *77*, 155-156.
4. Rioux, F.; DeKock, R. L. *J. Chem. Educ*. **1998**, *75*, 537-539.
5. Rioux, F. *J. Chem. Educ*. **1999**, *76*, 605.
6. DeKock, R. L. *J. Chem. Educ*. **1999**, *76*, 605-606.
7. *CRC Handbook of Chemistry and Physics*, 80th ed.; CRC: Boca Raton, FL, 1999; p. 12-15.
8. Burkert, U.; Allinger, N. L. *Molecular Mechanics*, American Chemical Society, Washington, D. C., 1982; p. 10.