

# letters

## Help Asked in Solving Ecological Education Problems in Byelorussia

To the Editor:

Within the past several years the world community has rendered great humanitarian assistance to the population of Byelorussia, including the Mogilev region, in overcoming the consequences of the Chernobyl catastrophe. The appalling consequences of radiation exposure has been aggravated by the complicated ecological situation that has arisen from unregulated development of the chemical industry and improper chemical application in agriculture.

These circumstances have awakened widespread chemophobia among the population. Nevertheless, the most reliable way of overcoming these complicated problems is through systematic education to prepare ecologically competent people to do the experimental work and apply it successfully and effectively in all branches of industry.

Unfortunately, our educational system has long produced the opposite—adults do not have the conviction that the majority of the necessary developments in our material, physiological, and social life must be based on changes coming from chemical science and technology. Naturally, changing this situation is possible only with daily, laborious, long-term, purposeful chemical education of our youth. For this purpose, the first Byelorussian Technological College was founded in Mogilev in 1990. The pupils with talent and inclination toward the natural and technical sciences are training here. The college has a chemical and technological department and a physical and mathematical department and matriculates 100 persons every year. The training process is directed toward a deep and active mastering of ecological knowledge. The professors and senior lecturers of the Mogilev Technological Institute take part in the training process. To graduate, the students must to know one foreign language (English or German) and be able to use the PC. The graduating students become laboratory assistants or PC operators.

We hope that the knowledge and the mode of education produces a deep understanding of the role chemistry and chemical technology play in the environment and that the graduating students play an important role in overcoming of our grave ecological situation.

We have supplied the College with modern computer engineering, so we have ensured a stable training process. At the same time, special chemical laboratories are necessary for teaching modern chemical methods. The laboratories should be equipped with modern instrumentation and plants; however, they are not available for purchase in our country, and we have no foreign currency. We temporarily carry out the training process in laboratories of the Mogilev Technological Institute. But their laboratories aren't supplied with modern equipment either.

Within the last two years humanitarian aid has been received by the Republic of Byelorussia from different countries. It's important. But the creation of a firm material base for our educational establishment, where the purposeful training of able people is begun, is more important. We appeal to our colleagues of different countries to help us to form the material and technical base of the Mogilev Technological College. We need your assistance in the purchase of complete chemical laboratories.

We would communicate to interested persons the list of chemical equipment and materials we need. We would be grateful for any contributions of literature on chemical educational and methodology (in English or German). It is also very important to establish constant contacts between Mogilev Technological College and analogous educational establishments in other countries, to organize interchange of teachers and students, etc.

Would those interested in helping please contact us at the address below.

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## A Revision of the Paper "Grid of Expressions Related to the Einstein Coefficients"

To the Editor,

J. E. Sturm [*J. Chem. Educ.* **1990**, *67*, 32] presents a grid of expressions in SI units relating the Einstein coefficients, oscillator strength, transition dipole moment, and integrated absorption coefficient for a transition between two states. The goal of the paper was praiseworthy and very useful because, as Sturm himself states, a problem situation arises for intermittent practitioners calling on a relation not developed explicitly in the given context, since some of those relations involve reconsideration of not only dimensional but also unit consistency. Effectively, to show the consistency of the expressions used by different textbooks in this context could be a formidable task due to the different notations and units employed and the not very unusual errors that appear in textbooks.

However, Sturm fails in his purpose because some inconsistencies have been introduced in the grid of expressions he suggests. For instance, the expression that relates the oscillator strength ( $f$ ) with the square of the transition moment ( $\mu^2$ ) is proposed to be:

$$f = \frac{(4\pi\epsilon_0)8\pi^2m\omega}{3\hbar e^2} \mu^2$$

The right term on this expression should be dimensionless since the oscillator strength is dimensionless. However, if you substitute each magnitude by its SI units you obtain  $C^2 \text{ kg J}^{-2} \text{ s}^{-1}$  units for the right term. In the same way, the relation between the Einstein coefficients,  $A$  and  $B$ , is proposed to be:

$$A = 8\pi\hbar c\omega^3 B$$

Units of  $\text{s}^{-1}$  and  $\text{s kg}^{-1}$  are obtained for  $A$  and  $B$ , respectively, in the worked example, where  $A$  and  $B$  are calculated by using the value of the integrated absorption coefficient,  $\int \epsilon d\omega$ . If you use these units for  $A$  and  $B$  and substitute the other magnitudes by their SI units you obtain the contradictory result  $\text{s}^{-1} = \text{s}$ . Similar inconsistencies are found in the expressions relating  $\int \epsilon d\omega$  and  $B$ ,  $\mu^2$  and  $A$ ,  $\mu^2$  and  $B$ , and  $\mu^2$  and  $\int \epsilon d\omega$ .

We believe that most of the inconsistencies observed in Sturm's paper result from the lack of universal criteria and the usual mistakes existing in the literature discussing the subject. For instance, J. M. Hollas (one of the authors referenced by Sturm) proposes the relation between  $A$  and  $B$  to be:

$$A = 8\pi h\omega^3 B$$

in his book *High Resolution Spectroscopy* (Butterworths, 1982; Chapter 2). In contrast, the same author proposes the relation to be:

$$A = 8\pi h c \omega^3 B$$

in his book *Modern Spectroscopy* (Wiley: New York, 1987; Chapter 2).

In the following table, we present a consistent grid of expressions relating the magnitudes discussed here. In these formulas, SI units are used for all the magnitudes including concentration ( $\text{mol m}^{-3}$ ). We have tried to be coherent with the notation used by Sturm. Anyway, a detailed explanation of the notation employed follows after the table. To derive the expressions appearing in the table, we have mainly used the book *Molecular Quantum Electrodynamics. An Introduction to Radiation-Molecule Interactions* by D. P. Craig and T. Thirunamachandran (Academic Press: New York, 1984). To our knowledge, this book represents one of the first attempts in using SI units to systematize quantum electrodynamics. The formulas presented here are also identical to those obtained by P. W. Atkins in *Molecular Quantum Mechanics* (Oxford University Press: New York, 1984).

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#### To the Editor:

I am grateful for the favorable response by Ortí and Planelles to the theme of my paper [1990, 67, 32]. We agree that a grid or table of expressions related to the Einstein coefficients is desirable. Their letter indicating errors was nevertheless disquieting since one tries to avoid errors especially in manuscripts for publication. My examples in the text of my paper are dimensionally correct for oscillator strength,  $f$ , dipole moment integral,  $\mu^2$ , and the Einstein  $A_{km}$  coefficient. We differ in two respects that affect some, but not all, of the relationships:

1. Dimensions of  $B_{km} = B_{mk}$ : One textbook (1) distinguishes  $B^0$  and  $B^1$ , which refer, respectively, to the energy density  $\rho$  and intensity  $I$ ;  $B^1 = B^0/c$ . In the original Einstein paper (2) only the  $B^0$  coefficient is used. My grid implicitly identifies  $B$  with  $B^1$ .

2. Use of  $(4\pi\epsilon_0)$ : Ortí and Planelles prefer to include explicitly this factor  $(4\pi\epsilon_0)$  in the expressions relating  $\mu^2$  to  $A$  and  $B$  and to the integrated absorption coefficient,  $\int \epsilon d\omega$ . An example in the text of my paper recognized the need for the factor; Ortí and Planelles have made the factor part of their grid.

Most disquieting, though, is my awareness of an inconsistency in my paper. My examples are dimensionally consistent with my definitions of terms. Some relations in the grid are, however, inconsistent with ones that would be derived from relations used in my examples. Let me be specific. In my example in the text, I use relations

$$\frac{f}{\int \epsilon d\omega} = \frac{(4\pi\epsilon_0)c^2 m_e \ln 10}{\pi q^2 N_0}$$

and

$$\frac{B}{\int \epsilon d\omega} = \frac{\ln 10}{h\omega N_0}$$

The ratio of these expressions would be

	A	B	$\int \epsilon d\omega$	$f$	$\mu^2$
A	1	$\frac{B}{A} = \frac{1}{8\pi h\omega^3}$	$\frac{\int \epsilon d\omega}{A} = \frac{N_0}{8\pi\omega^2 \ln 10}$	$\frac{f}{A} = \frac{(4\pi\epsilon_0)mc}{8\pi^2 e^2 \omega^2}$	$\frac{\mu^2}{A} = \frac{(4\pi\epsilon_0)3h}{64\pi^4 \omega^3}$
B		1	$\frac{\int \epsilon d\omega}{B} = \frac{N_0 h \omega}{c \ln 10}$	$\frac{f}{B} = \frac{(4\pi\epsilon_0)mch\omega}{\pi e^2}$	$\frac{\mu^2}{B} = \frac{(4\pi\epsilon_0)3h^2}{8\pi^3}$
$\int \epsilon d\omega$			1	$\frac{f}{\int \epsilon d\omega} = \frac{(4\pi\epsilon_0)mc^2 \ln 10}{\pi e^2 N_0}$	$\frac{\mu^2}{\int \epsilon d\omega} = \frac{(4\pi\epsilon_0)3hc \ln 10}{8\pi^3 \omega N_0}$
$f$				1	$\frac{\mu^2}{f} = \frac{3he^2}{8\pi^2 mc\omega}$
$\mu^2$					1

$\omega = 1/\lambda$  ( $\text{m}^{-1}$ ), where  $\lambda$  is the wavelength of the transition.

$A = A_{mk}$  ( $\text{s}^{-1}$ ) is the first-order rate coefficient for spontaneous emission between states  $m$  and  $k$ .

$B = B_{mk}$  ( $\text{J}^{-1} \text{m}^3 \text{s}^{-2}$ ) is the rate coefficient for stimulated transition.

$\epsilon$  ( $\text{mol}^{-1} \text{m}^2$ ) is the extinction coefficient defined from the Lambert-Beer law  $I = I_0 10^{-\epsilon \eta z}$ . Here  $\eta$  ( $\text{mol m}^{-3}$ ) represents concentration and  $z$  (m) path length. The natural form of the Beer law is  $I = I_0 e^{-\alpha \eta z}$ . Thus,  $\alpha$  is related to  $\epsilon$  by the expression  $\alpha = \epsilon \ln 10$ .

$f$  (dimensionless) is the oscillator strength.

$\mu = \mu_{km}$  (C m) is the transition dipole moment.

$h$  (J s) is the Planck constant.

$N_0$  ( $\text{mol}^{-1}$ ) is Avogadro's number.

$c$  ( $\text{m s}^{-1}$ ) is the speed of light.

$e$  (C) is the electron charge.

$m$  (kg) is the electron mass.

$(4\pi\epsilon_0)$  ( $\text{J}^{-1} \text{C}^2 \text{m}^{-1}$ ) is the rational factor of the SI unit system.

$$f/B = (4\pi\epsilon_0)^{-1} c^2 m_e h \omega / (\pi q^2)$$

which would be in agreement with Ortí and Planelles' expression.

Unfortunately, my grid has  $c$  instead of  $c^2$  for this ratio even though the expression for  $B/f$  on the grid has  $c^2$  as do Ortí and Planelles. All I can do now is to acknowledge this inconsistency.

To complete the package, four typographical errors might as well be noted.

1. On the grid, in the expression for  $f/B$ , the symbol  $\xi$  is used instead of the intended  $q$ , the electron charge.
2. Also on the grid, the "y" is missing from  $\mu^2/f$ .
3. The last sentence of the first paragraph on p 33 has the word "dimensionless" misspelled "dimensionsless".
4. In the denominator of the long numerical expression for  $f$ , the unit C (for coulombs) is missing from the magnitude of  $q$ .

The ultimate outcome of this somewhat less-than-fulfilling experience hopefully is a correct set of relations among these fundamental and important terms. I thank Ortí and Planelles for offering their corrected form of the grid.

#### Literature Cited

1. Steinfeld, J. I. *Molecules and Radiation*, 2nd ed.; MIT Press: Boston, 1985; pp 27 ff.
2. Einstein, A. *Physik. Zeitsch.* 1917, XVIII, 121-128.

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#### Putting Some Snap into Work

To the Editor:

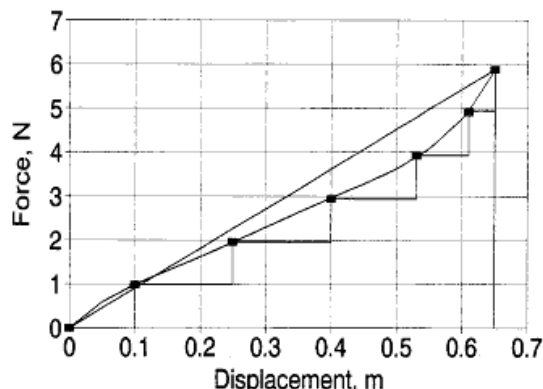
The *Tested Demonstration* "Maximum Work" by John Salzsieder [1990, 67, 962] very cleverly illustrates the concept of reversible work. I have several suggestions that I think can add to its instructional value.

With rubber bands, the relationship of force and displacement is not, as Salzsieder notes, a linear one. To estimate the reversible work, Salzsieder uses a linear approximation of this relationship. One can use a spring as an alternative to rubber bands; if one takes care to see that the coils do not come into contact at the smallest extension used, the relationship of force and displacement is linear (following Hooke's law), and the calculation of reversible work gives a precise value.

There are advantages to using rubber bands, however. If one stretches a rubber band and quickly touches it to the lips, a slight warming can be felt; if one then unstretches the rubber band and again touches the lips, a slight cooling is apparent. A few cycles of this process serve to demonstrate quite convincingly that contraction of a rubber band is an *endothermic* process. This means that the contraction of a rubber band, a spontaneous process, is *not* driven by a decrease in potential energy, but by an increase in entropy. This counterintuitive demonstration provides a good introduction to the meaning of the Gibbs free energy function.

A further advantage of rubber bands is the nonlinear force-displacement relationship, for it leads to a more general appreciation of the representation of work as the area under a force versus displacement curve. One can use the experimental data and numerical integration to arrive at a more precise result for the reversible work.

The figure illustrates one way in which this may be done. In this graph, the seven points plotted are based on data from Salzsieder's article. The curve connecting the data points was generated by fitting a fifth-order polynomial in displacement to the experimental data, then using the re-



Force vs. displacement for a rubber band (data from Salzsieder [1990, 67, 962]).

sulting equation to calculate interpolated values at 0.05-m intervals. Piecewise calculation of the area under this curve gives a value of 1.65 J for the reversible work. This value may be compared with the estimate of 1.91 J for reversible work calculated with a linear approximation, corresponding to the area under the line drawn between the first and last points on the graph. The area under the step function in the figure represents the work available if the six 100-g masses are removed one at a time; the total work for this process is 1.33 J.

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#### Argon-Potassium Atomic Weight Inversion in the Periodic Table

To the Editor:

In evolving his periodic classification of elements in the order of increasing atomic weights ( $A$ ), Medeleeff had to reverse the order at two places, bringing Co ( $A = 58.9332$ ) before Ni ( $A = 58.7100$ ) and Te ( $A = 127.600$ ) before I ( $A = 126.9044$ ). Subsequently, when Ar ( $A = 39.9480$ ) was discovered it had to precede K ( $A = 39.1020$ ). These constitute three exceptions in the order of atomic weights. When the phenomenon of isotopy was understood, it was realized that the atomic weight of a naturally occurring element is just the weighted mean of the atomic masses of the isotopes making it up. However, as the number of stable isotopes of an element, as well as their relative abundances varied randomly over wide limits from element to element, atomic weights ceased to be of significance in characterizing elements, and the three exceptions in the periodic table came to be accepted as a fortuitous fact though of no importance. Still it is a curious fact that amongst the hundred odd elements there should be only three exceptions unexplained so far.

In the case of the Ar-K inversion, however, an explanation seems to be available in the nuclear characteristics of the naturally occurring isotopes of these elements, which are both triisotopic with following atom percent abundances.

$$^{36}\text{Ar} = 0.34\%; \quad ^{38}\text{Ar} = 0.06\%; \quad ^{40}\text{Ar} = 99.6\% \\ ^{39}\text{K} = 93.22\%; \quad ^{40}\text{K} = 0.012\%; \quad ^{41}\text{K} = 6.77\%$$

of these nuclides, only  $^{40}\text{K}$  is radioactive decaying by  $\beta^-$  (88.8%) to  $^{40}\text{Ca}$  and by EC (11.2%) to  $^{40}\text{Ar}$ . Geochemists