### AN ABSTRACT OF THE THESIS OF

<u>Lawrence D. Fields</u> for the degree of <u>Master of Science</u> in <u>Chemistry</u> presented on <u>November 7, 1985</u>.

Title: <u>Some Recent Developments in the Theory of Significant Figures</u> and their Applications to Chemical Instrumentation

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Significant figures have been a nebulous area in the physical sciences. The results of a literature survey, and of a questionaire distributed among the Chemistry Department faculty at Oregon State University, revealed widely differing interpretations regarding the proper role of significant figures. The present study has a two-fold nature.

First the existing theory was extended to include the Root Rule, which unambiguously assigns the correct number of significant figures to the result of a chemical or physical calculation.

Then significant figure theory was applied in developing improved methods for recording (and transmitting) tables of measurement data. The upshot is two novel data compression techniques—Decimal Coded Binaries (DCB) and Eight Code—which efficiently combine a measurement and its uncertainty into a single number.

An investigation of the computer interfacing requirements of DCB and of Eight Code vis-a-vis a pH meter and a spectrophotometer demonstrated that these new communications tools are easily implemented. <sup>C</sup> Copyright by Lawrence D. Fields November 7, 1985

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Some Recent Developments in the Theory of Significant Figures and their Applications to Chemical Instrumentation

by

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# SOME RECENT DEVELOPMENTS IN THE THEORY OF SIGNIFICANT FIGURES AND THEIR APPLICATIONS TO CHEMICAL INSTRUMENTATION

### INTRODUCTION

Significant figures have long been a delinquent stepchild of the physical sciences. Not only is there a paucity of literature on the subject, but the results of an informal survey of the Chemistry Department faculty at Oregon State University indicates a polarization of views on the proper use of significant figures. Thus significant figures have been elevated to the status of a sacred cow. As with most sacred cows, there is a consensus on the sacredness, but the nature of the cow is not clear. We need a more cogent theory of significant figures.

If the components of a calculation are represented by **stand-alone significant figures** (measurement-based quantities, for which the uncertainties are not given directly, and must be inferred from the number of significant figures used to represent them), then we should be able to represent the result of the calculation in the same way. We will see that the **Root Rule** (described herein), unlike previous significant figure rules, successfully integrates common arithmetic operations with propagation-of-uncertainty analysis, thereby providing a sensible and unambiguous criterion for deciding how many digits should be used to represent the result of any calculation in the physical sciences.

However the utility of the theory is limited by the number system being used. Because of our ten fingers, the estimated uncertainty of a quantity represented by stand-alone significant figures can be resolved only within a ten-fold range. Would some other number system be better?

If we ignore the fact that binary numbers take up so much space, we might do well to adapt the theory of significant figures to the base two number system. Then the uncertainty of a quantity represented by stand-alone significant figures could be pinned down within a two-fold range. Fortunately it is possible to construct a nomenclature which incorporates this virtue of binary into the base ten number system, a completely new application of significant figure theory.

In this new approach, two number systems are combined in order to incorporate two types of information—a measurement and its uncertainty—into a single number. The result is a format, which looks and reads like ordinary base 10, and which gives the same information about uncertainty as binary. This type of nomenclature is called **Decimal Coded Binaries (DCB)**.

One possible application of DCB would be in the reporting of tables of measurement data. If a table has a DCB format, then reporting the uncertainty of a measurement along with the measurement itself will be economical, and will not decrease the readability of the table.

However DCB may have a larger impact in the area of data compression and transmission. Using DCB, a collection of measurement data can be stored more compactly in memory devices, and can be telecommunicated with greater efficiency, than would be the case if each measurement and its uncertainty were treated as two separate numbers.

There is a second data compression technique, called Linear Code, which is very simple. Linear Code serves primarily as a auxiliary technique, which helps to clarify DCB and its advantages. Moreover Linear Code can be hybridized with DCB. Therefore Linear Code is included as a section in the chapter on DCB.

The bulk of this thesis (which uses the optional publication format) consists of two papers on stand-alone significant figures and on DCB (with Linear Code). The first has been accepted for publication in the Journal of College Science Teaching. The second has been submitted for publication to Analytical Chemistry. The thesis also contains some material (like Eight Code), which has not been submitted for publication.

Just as DCB combines two number systems (2 and 10) in order to compress a measurement and its uncertainty into a single number, a third technique—Eight Code—accomplishes the same objective, using three number systems (2, 4, and 10). At one point in our investigation, Eight Code was a competitor of DCB. However mature consideration showed that Eight Code is a prototype for a more sophisticated approach (combining N number systems), which is beyond the scope of the present research. Here we will consider only data compression techniques which can be programmed into an HP15C scientific calculator. Listings of these programs are also included. All three techniques are original.

DCB has commercial implications. If DCB becomes generally accepted, then scientific calculators will have to be redesigned to accomodate DCB coding and decoding routines, as well as DCB arithmetic, which will draw upon the Root Rule concept. Moreover computer languages used in scientific work may need a new type of declaration for DCB variables, in addition to the usual integer and floating point variables.

# SIGNIFICANT FIGURE FUZZINESS IS MINIMIZED WITH A ROOT TEN RULE.

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### PART I: MULTIPLICATION AND DIVISION

#### Introduction.

"Why it's perfectly obvious!" "It's just a matter of common sense." These are typical responses to the question of how many significant figures should be used to express the result of a calculation in the physical sciences. In an attempt to measure the ubiquity of such common sense, we conducted an informal survey of the Chemistry Department faculty at Oregon State University. Each participant was given a questionaire, which asked him or her to write the following product with the proper number of significant figures:

1.43 \* 4.098 = 5.86014

Only one fifth of the respondents answered correctly.

In all fairness, we must add that one third of the respondents had reasonable complaints about ambiguity in the question. Even so, our questionaire indicated that "significant figure" is similar to "democracy", in the sense that both concepts mean different things to different people.

This type of question, and the confusion it engenders, is the <u>raison</u> <u>d'etre</u> for this paper. Some scientists would like to pontificate **stand-alone significant figures** out of existence. Yet significant figures are mentioned in the first chapter of many general chemistry and general physics texts, and are often a sub-problem in undergraduate lab reports (and in the real world). Since stand-alone significant figures are a fact of life, it would behoove us to treat them systematically.

It has been said that a teacher should be like an iceberg, in the sense that 90% of the essence is beneath the surface. In accordance with this philosophy, we are attempting a two-fold education project. First we seek to give the teacher a solid understanding of the theory of significant figures, with special emphasis on calculations in which the component uncertainties are not given directly. This will be the main thrust of Part I, whose cornerstone is the **Root Rule** for multiplication and division calculations, having a single identifiable **least precise factor**.

Moreover we have distilled some teachable significant figure algorithms (both of which are based upon the Root Rule), which should be appropriate for college-level courses in chemistry and physics. For teachers, the most pertinent results are the **Three Rule** and the **1–5 Rule** in Part I, which also contains a section on "Significant Figures and Science Education".

We are not attempting to usurp the role of rigorous uncertainty analysis; rather our topic is a specialized area within this broader field. The basic idea of this paper is that the number of significant figures used to express the product or quotient of a physical science calculation should reflect the fact that the percent uncertainty of the result will be approximately equal to percent uncertainty of the least precise factor.

Part I is addressed largely to college science educators seeking useful and teachable knowledge to impart to their students. Part II is more comprehensive, and uses more complicated procedures (all of which can be written into computer programs). It is of interest to the scientific generalist within each of us (and to the manufacturers of computers, scientific instruments, and calculators).

A survey of the literature on significant figures suggests that Newton's giants are relatively few in number, and that they have rather narrow shoulders. This gives us the opportunity to explore more than the unusual amount of virgin territory in this paper. Uncertainty is a key concept in the theory of significant figures. There are two main reasons why we might feel uncertain about a reported measurement which we encounter in the literature.

- Systematic error (sometimes called determinate error). Skoog and West<sup>1</sup> have delineated the following three categories of systematic error:
  - (a) personal error (such as a number bias on the part of the experimenter)
  - (b) instrumental error
  - (c) method error
- Random error (also known as indeterminate error or imprecision). If the random error is large then the meaurement is not very reproducible.

Now that we have mentioned some of the sources of **measurement uncertainty**, we need to define the term. For the sake of simplicity, we will consider only two of the more popular definitions of uncertainty.

A. Uncertainty is the <u>absolute limit of error</u>. This definition is easy to understand, and is the raw material for the worst case method<sup>2</sup> of uncertainty analysis. Definition A has the advantage of taking both random and systematic errors into account.

However this definition has very limited utility in the real world. The absolute limits of error are often unknown and/or unknowable. Moreover if the random errors are normally distributed, as we so often assume, then the absolute limits of error don't even exist!

B. Uncertainty is the <u>sample standard error of the mean</u>  $(s/\sqrt{N})$  for a series of measurements, or the <u>population</u> standard deviation ( $\sigma$ ) for a single measurement. Unlike A above, this definition applies to the real world, since the standard error of the mean can be calculated quite readily. The standard error definition is especially useful

when the systematic error is thought to be negligible in comparison with the random error. However the standard error of the mean says nothing about systematic error.

In the remainder of Part I, we will use Definition B for two reasons. First, the standard error of the mean is the more sensible definition. Secondly, we will introduce some vest-pocket algorithms (like the 1-5 Rule) which are not always appropriate for the absolute limit of error definition of uncertainty.

In Part II, we will extend our approach to include significant figure determinations for functions of n variables. In the more general case, the equation for propagation of uncertainty will depend upon the definition of uncertainty. We will favor the standard error of the mean definition.

We have already mentioned that the percent uncertainty implied by the number of significant figures used to represent the product or quotient of a physical science calculation should be in the same ballpark as that of the least precise factor. In the next two sections we will develop some concepts, which will enable us to see why the traditional approach to significant figures does not fully come to grips with this important idea. There is a consensus among physical scientists that the reporting of a measurement should include at least the following two components:

1) the measurement itself

an estimate of the measurement's uncertainty.

Sometimes the estimated uncertainty is given indirectly in terms of the number of significant figures in a measurement-based quantity. In the following discussion, "±" will denote the uncertainty.

There seem to be four main schools of thought about the meaning of significant figures. The Conservatives insist that the last significant figure must be known with certainty. For example, a measured value of 1.43 is understood to mean  $1.43 \pm 0.005$  at the worst. In essence, the Conservative is saying, "I want information I can trust."

The Mainstreamers believe that there can be appreciable uncertainty only in the last significant digit, but there is disagreement about how much uncertainty is allowed in the last digit  $(\pm 1, \pm 2, \pm 3, \text{ etc.})$ .

The Liberals feel that there can be appreciable uncertainty in the last <u>two</u> significant digits. The liberal is saying, "I want the maximum amount of useful information."

The central concepts of this paper will be illustrated using the Mainstream approach. However little generality would be lost if the Liberal approach were used instead. We should mention one final school of thought about significant figures.

The Independents are of the opinion that significant figures should never be used <u>by themselves</u> to indicate an estimated uncertainty. However there is a major problem with the Independent position. Organic chemists do not always report ± values for percent yields. Physicists and analytical chemists do sometimes omit uncertainties from data tables. In the real world, stand-alone significant figures are often used to indicate (in a round-about way) the uncertainty of measurement-based quantities. However this usage has not been very systematic.

In some instances it is reasonable to allow stand-alone significant figures to supplant directly reported uncertainties. In data tables reported uncertainties take up extra space, and can decrease readability. Moreover, if a chemical analysis is performed on only two or three samples drawn from a large population, then the direct reporting of the uncertainty may be slightly presumptuous.

When the uncertainties of the components in a calculation are available, it is a relatively simple matter to assign what one considers to be the correct number of significant figures. Significant figures are fuzziest when they stand alone, when ± values are not available. In this paper, we are mainly concerned with these fuzzy significant figures. Another important source of significant figure fuzziness is politics.

Influential laymen may insist on knowing the results of scientific measurements in very simple terms. This can result in politically motivated biases and double standards with respect to significant figures. The number of significant figures assigned to a quantity may depend on its intended use. If a result will be used by decision-makers who will not understand its uncertainty, or while understanding, will ignore it for political reasons, while blaming the writer for any unfortunate consequence, then it is better to round, such that the last reported digit can be rigorously defended. If the decision-maker needs the most detailed information and understands its limitations, then uncertainty in the last two digits may be justified.

Sometimes a writer's intention is simply to give the reader a general feeling for the magnitude of a quantity. Often two or three significant figures are sufficient for this purpose, even though four might be scientifically justifiable. In the remainder of this paper, we will try to ignore such political considerations.

There is an obvious lack of consensus on the meaning of stand-alone significant figures. However we will formulate valid significant figure rules which are relatively independent of ± conventions.

We will tentatively assume, without loss of generality, that the final significant digit in an inexact number (i.e. a measured value) can readily be one higher or one lower than face value. For example, "7.2" is understood to mean "7.2  $\pm$  0.1". The "0.1" is the **implied uncertainty**. The **implied relative uncertainty** is 0.1/7.2 = 1/72.

It would be nice if the number of significant figures in a product (or quotent) could be adjusted such that the implied relative uncertainties of the product and of the least precise factor are equal. However this is usually impossible to do. In the general case, one of two things is done: 1) Make a seat-of-the-pants judgment.

2) Apply a significant figure algorithm.

Of course no significant figure algorithm can exist in a vacuum. It must be consistent with propagation-of-uncertainty analysis. In our earlier example

"1.43" has a larger implied relative uncertainty than "4.098". Thus "1.43" is the **least precise factor**. In general the least precise factor is the factor with the least number of significant figures.

Exact numbers, which come from definitions and from ordinary counting, have infinitely many significant figures. For example in the kinetic energy formula,

the "0.5" can never be the least precise factor.

If two factors have the same number of significant figures, then the least precise factor is the one whose **mantissa**<sup>\*</sup> is the smaller of the two. However in this case, we should bear in mind that both factors will contribute an appreciable amount of uncertainty.

As a first approximation, we can usually ignore the uncertainty contribution made by the other factor. In this case, it is intuitively obvious that the relative uncertainty of the product should approximate the relative uncertainty of the least precise factor. This fact is the basis for the significant figure algorithms of Part I.

<sup>\*</sup>For example in  $3.45 \times 10^{-2}$  the "3.45" is the mantissa.

The **Textbook Rule** for significant figures in multiplication and division, usually given in physics and chemistry texts is similar to the following:

The number of significant figures used to express a product or quotient <u>should not exceed</u> that of the least precise factor.

However this begs the question. The rule which is actually taught is usually similar to the following **Simple Rule**.

The number of significant figures in a product or quotient is equal to that of the least precise factor.

(Note that the Conservative approach is the tacit frame of reference for the first Textbook Rule, while the second Simple Rule is consistent with both the mainstream and Liberal aproaches.)

The Simple Rule carries with it four implicit assumptions:

- 1) A single least precise factor exists.
- 2) The ± value is not known, but the same ± convention applies in determining the uncertainty of each factor. (For instance the 1.43 and 4.098 in our example can have uncertainties of 0.01 and 0.001 respectively, or 0.02 and 0.002, but not 0.01 and 0.002.) Thus the least precise factor can be readily identified.
- 3) The least precise factor is the only significant source of uncertainty in the product.
- 4) The ± convention is not smaller than about ±1. (See Part II)

We will see that even when these criteria are met, the Simple Rule frequently gives absurd results.

Pinkerton and Gleit<sup>3</sup> have taken a more sophisticated approach. They argue that the number of significant figures in a quantity is logarithmically related to the reciprocal of its relative uncertainty. Although this helps to clarify the concept of significant figures, it has little to say about the practical problem at hand.

In the next section we will carry this concept to its logical conclusion, by introducing the **Root Rule** for significant figures in multiplication and division, which is the basis for the methods used in the General Chemistry program at Oregon State University.

### The Root Rule

A significant figure algorithm should be unbiased. If the algorithm has an optimistic bias, then the accuracy of one's measurements is exaggerated. A pessimistic bias means that information is being thrown away unnecessarily. The Simple Rule, as applied to the Mainstream and Liberal approaches, is essentially unbiased when it is used correctly. However it has boundary condition problems, which we will illustrate using the following **1–9 Paradox**. Consider the division calculation:

1.01/1.020 = 0.990196

According to the Simple Rule, the quotient should be written as 0.990 (three significant figures). The implied relative uncertainty of this number is calculated as follows:

0.001/0.990 = 1/990 = 0.1%

The implied relative uncertainty of the least precise factor is:

The two implied relative uncertainties differ by nearly an order of magnitude (a factor of ten). A more sensible answer would be 0.99, since the implied relative uncertainties of both quotient and least precise factor would be about 1%. Now we will develope the conceptual framework for an algorithm which does not lead to such absurdities.

Let P be the implied relative uncertainty of the product (or quotient), which has been tentatively rounded according to the Simple Rule, and let L be that of least precise factor. By adjusting the number of significant figures used to express the product (or quotient), we can manipulate P, such that P is as close (in a logarithmic sense) to L as possible. But how close is possible in the general case? According to the Simple Rule, it is always possible to adjust P, such that

If the product (or quotient) is rounded to one less digit than this, then the implied relative uncertainties will be L and 10 P. Usually either P/L or 10 P/L will be nearer to one. In the borderline case,

and solving for P/L yields

$$P/L = 1/\sqrt{10}$$

When the product (or quotient) is given one <u>more</u> significant figure than the Simple Rule would suggest, the two implied relative uncertainties will be L and 0.1 P. Now there is the possibility of a second type of borderline case in which

$$\frac{P}{L} = \frac{L}{0.1 P} = \sqrt{10}$$

This then is the framework mentioned above for the result, which is discussed below as the LPF Root Rule (LPF = least precise factor). Our two borderline cases lead us to the following rule for significant figures in multiplication and division.

The LPF Root Rule: If the uncertainties are not given, and if

$$\frac{1}{\sqrt{10}} < \frac{P}{-} < \sqrt{10}$$

then the product (or quotient) has been rounded to the correct number of significant figures. (The same four restrictions, which apply to the Simple Rule, also apply to the LPF Root Rule.)

The Simple Rule allows an implied relative uncertainty discrepancy of nearly an order of magnitude in either direction. The LPF Root Rule says that this is too much, that the discrepancy should be no more than half an order of magnitude.

We will return to our original example in order to illustrate the LPF Root Rule. We will also show that the LPF Root Rule is quite general, and is relatively independent of  $\pm$  convention (provided that it is not too small).

1.43 \* 4.098 = 5.86014

First we will use the ±1 convention. The implied relative uncertainty of 1.43 is 0.01/1.43 = 1/143. The implied relative uncertainty of 5.9 is 0.01/5.9 = 1/59.  $1/59 \div 1/143 = 143/69 = 2.42 < \sqrt{10}$ Therefore the product has been correctly rounded to 5.9.

Note that the implied relative uncertainties of least precise factor and product differ by log 2.42 = 0.38 of an order of magnitude. It is the best we can do in this example, as we will see in the next paragraph.

Suppose that the product had been rounded to 5.86 (three significant figures) instead. The implied relative uncertainty of 5.86 is 0.01/5.86 = 1/586. The new implied relative uncertainty ratio would be

and the implied relative uncertainties of least precise factor and

product would differ by log 4.1 = 0.61 of an order of magnitude (as compared with 0.38 of an order of magnitude for two significant figures). Thus "5.9" is the lesser of two evils.

This result is not affected if some other ± convention is used instead of ±1. To demonstrate this, we will apply a ±2 convention. The implied relative uncertainty of 1.43 is 0.02/1.43 = 2/143. The implied relative uncertainty of 5.9 is 0.02/5.9 = 2/59.  $2/59 \div 2/143 = 143/59 = 2.42 < \sqrt{10}$ 

Therefore our approach really is "without loss of generality". This makes the LPF Root Rule relatively independent of  $\pm$  convention, provided that all of the inexact numbers used in the original calculation follow the same  $\pm$  convention. There is no a priori way to know that this will be true, but it is the only assumption we can make if the uncertainties are not given directly. We leave it as an exercise for the reader to show that the LPF Root Rule leads to the correct number of significant figures in the 1–9 Paradox (1.01/1.020 = 0.990196).

The LPF Root Rule says that in most cases we can (and should) adjust the number of significant figures in the product or quotient such that uncertainty in the final digit of the product or quotient is 0.3162 to 3.162 times the uncertainty of the final digit of the least precise factor---even though we do not know what this latter uncertainty is!

In terms of the Pinkerton-Gleit definition of significant figures, the LPF Root Rule says that a product or quotient has been rounded correctly if it is within  $\pm 0.5$  significant figures of the least precise factor, i.e. if

 $\left| \log \frac{1}{\frac{1}{\text{IRU (LPF)}} - \log \frac{1}{\frac{1}{\text{IRU (result)}}} \right| < 0.5$ 

where **IRU** represents "the implied relative uncertainty of", and **LPF** represents "the least precise factor".

Sometimes either rule may seem either too optimistic or too pessimistic to an outside omniscient observer. However the Root Rule is a reasonable and unambiguous method for significant figure determinations, when the component uncertainties are not known. Another limitation of the LPF Root Rule will be illustrated with the following example:

2 X 4.4 = 8.8 which rounds to 9

The least precise factor "2" has only one significant figure. According to the LPF Root Rule, the number of significant figures in the product should be one less than this, or zero, which is absurd. The best we can do is to round the product to 9.

One-significant-figure-quantities can be quagmires of uncertainty, especially in subtraction calculations, involving two nearly equal quantities, each having appreciable uncertainty. In such cases ± conventions have little meaning.

The LPF Root Rule for significant figures is a right-brain approach, which may not be suited to left-brain people. Therefore we will give some equivalent formulations and approximations to the Root Rule. The casual reader should choose the most comfortable of these new rules, rather than trying to master and to remember all of them. (We recommend either the 1–5 Rule or the Three rule, given in the next two sections.) For the benefit of computer programmers, the LPF Root Rule may be expressed by the following LPF Root Rule Algorithm:

- 1) Express all numbers in scientific notation. For example, 0.0345 is  $3.45 \times 10^{-2}$  in scientific notation. The 3.45 shall be called the **mantissa**.
- 2) Find the least precise factor.
  - A. The least precise factor is the factor with the least number of significant figures.
  - B. If two factors have the same number of significant figures, then the least precise factor is the one whose mantissa is the <u>smaller</u> of the two. (Strictly speaking, neither the Simple Rule nor the LPF Root Rule applies in Case B, since the least precise factor does <u>not</u> contribute essentially all of the uncertainty. If we want to avoid introducing an optimistic bias into our results, then we must use the methods of Part II.)
  - C. Obviously an exact number cannot be the least precise factor because an exact number has infinite precision.
- 3. Compare the mantissas of the answer and of the least precise factor.

- A. Divide the larger mantissa by the smaller mantissa.
- B. If this quotient is less than  $\sqrt{10}$ , then the answer will have the same number of significant figures as the least precise factor.
- C. If the quotient is √10 or more, then adjust the number of significant figures in the answer mantissa, such that the smaller mantissa has one more significant figure than the larger mantissa. (Do not give the answer mantissa less than one significant figure.)

It can be shown that the LPF Root Rule over-rides the Simple Rule about 25% of the time in two-factor multiplication and division calculations. This means that when the component uncertainties of a multiplication or division calculation are <u>not</u> known, the Simple Rule can be expected to give unreasonable results (as in the 1–9 Paradox) about one fourth of the time. (See Appendix.)

The LPF Root Rule and the above algorithm are too complicated for most general chemistry students. In the next section, we will derive a simplified procedure. The purpose of this section is to develop the 1–5 2–8 Rules, two 'quick and dirty' rules of thumb for the LPF Root Rule. In particular, the 1–5 Rule is easy to apply, easy to remember, and very useful. But first we must introduce an intermediate result, which follows from the LPF Root Rule. The starting point for the 1–5 2–8 Rules is the following 1–7 Rule.

The Simple Rule does <u>not</u> apply when the least precise factor begins with a "1", and the product or quotient begins with "7", "8", or "9" (or vice versa). In this case, the quantity beginning with "1" should have one more significant figure than the other quantity. As a mnemonic, we can say, "One gets one more." (Remember that a quantity cannot have less than one significant figure.)

The 1-7 Rule is justified as follows:

- 1) For the borderline case in which the 1-7 Rule barely over-rides the Simple Rule, the mantissas of the two numbers will be 1.999 and 7.00.
- 2)  $7.00/1.9999 = 3.5 > \sqrt{10}$
- 3) Therefore by the Root Rule, the correct number of significant figures has been assigned.

We have seen that the 1-7 Rule is always correct when it supersedes the Simple Rule. However it doesn't supersede often enough. The 1-7 Rule lacks comprehensiveness. In the next few paragraphs, we will argue that the following procedure would be better than the 1-7 Rule. The 1-5 2-8 Rules:

- A. If the least precise factor begins with a "1" and the product or quotient begins with "5", "6", "7", "8", or "9" (or vice versa) then give the quantity beginning with "1" one more significant figure than the othere quantity. (Mnemonic: one gets one more.)
- B. If the least precise factor begins with a "2" and the product or quotient begins with "8" or "9" (or vice versa) then give the quantity beginning with "2" one more significant figure than the other quantity.
- C. If neither A nor B applies then use the Simple Rule.
- D. The product or quotient must have at least one significant figure.

For purposes of the 1-5 2-8 Rules, the first digit of a quantity is never zero. For example, the number 0.05916 is said to begin with a "5".

The original 1-7 Rule has annexed four new combinations: "1-5", "1-6", "2-8", and "2-9". Unlike the original 1-7 Rule, the 1-5, 2-8 Rules sometimes supersede the Simple Rule when they shouldn't. However they are in closer agreement with the Root Rule. Let's see why this is so.

Let the **critical numbers** of a multiplication (or division) calculation be defined as the mantissas of the least precise factor and of the product or quotient. In order to illustrate our approach, we'll look at the marginally useful 1–5 combination. The lower critical number begins with a "1", and the higher with a "5". If the lower critical number is less than

then the 1-5 Rule will agree with the LPF Root Rule. We will illustrate this point with two borderline cases. In the following example:

the two critical numbers are 1.58 and 5.0007. Since they differ by a factor of 3.165, which is <u>barely</u> greater than  $\sqrt{10}$ , the LPF Root Rule and the 1–5 Rule barely agree that the product should be rounded to 5.0. In the following example, the two rules will <u>barely</u> disagree:

(Use a similar line of reasoning.)

The 1-5 Rule and the LPF Root Rule <u>sometimes</u> agree when the lower critical number is greater than 1.581, but less than

$$5.999/\sqrt{10} = 1.897$$

as shown by the following example:

1.89 **\*** 3.174 = 5.99886

in which both rules agree on "6.0".

Thus we would expect the 1-5 combination to conform to the LPF Root Rule in more than 58% (because of the "58" in our magic number, 1.581) of all possible cases for a given number of significant figures.

Now here is the other side of the coin. Suppose that we had used the 1-7 Rule. Since the 1-7 Rule does not cover the 1-5 combination, the Simple Rule would apply. Loosely interpreted, the above argument says that this would be wrong more than 58% of the time. Similar arguments can be constructed for the 1-6, 2-8, and 2-9 combinations.

If one had to choose the single most important thing to remember from this paper, then either the 1-5 Rule or the Three Rule (given in the next section) would be that choice. The 1-5 Rule is nice in the following ways:

(a) It is easy to apply and to remember.

(b) It rectifies the most blatant absurdities of the Simple Rule.

## The Three Rule

The pedagogical weakness of the 1-5 Rule is that it is a magic formula; it gives no insight into the concept of keeping track of uncertainties in a calculation. For this reason we have developed the Three Rule, which places greater emphasis on propagation of uncertainty than either the Root Rule (on which it is based) or the 1-5 Rule.

The Three Rule:

- A. Locate the least precise factor. Calculate its relative uncertainty using the ±1 convention.
- B. Convert the product or quotient to scientific notation, and multiply its mantissa by the relative uncertainty. This is the <u>uncertainty of the product mantissa</u>.
- C. Note the position (relative to the decimal point) of the first (nonzero) digit in the uncertainty of the product mantissa. <u>Tentatively</u> assume that the last significant digit of the product mantissa will be in the same position.
- D. Note the value of the first (non-zero) digit in the uncertainty of the product mantissa. If it is "1" or "2", everything is OK. Otherwise if it is "3" or more, then round off one more digit. (The rounded product or quotient must have at least one significant figure.)

As an example, let's use the Three Rule to round the product in our original problem:

- A. The least precise factor is 1.43. It's implied relative uncertainty is 0.01/1.43 = 1/143
- B. Uncertainty of the product mantissa = (1/143) \* 5.86014 = 0.04098
- C. The uncertainty is in the hundredth's place of the product mantissa.
- D. The number in the hundredths' place (4) is not 1 or 2. Therefore we can only write the product mantissa with one significant digit after the decimal point. When properly rounded, the product is 5.9.

The Three Rule is slightly pessimistic, which allows for a significant contribution of uncertainty from factors other than the least precise factor. Unlike the 1-5 Rule, the Three Rule helps the user to develop the knack for keeping track of uncertainties in a calculation. The Three Rule is more comprehensive, but less facile than the 1-5 Rule.

### Significant Figures and Science Education

Since 1981, the rudiments of significant figure theory have been taught in Chem. 104 at Oregon State University. Chem. 104, 105, 106 is the lower track General Chemistry sequence (for students whose high school backgrounds are weak in terms of chemistry and mathematics). Both the 1–5 Rule and the Root Rule Algorithm have been used at different times.

The Root Rule Algorithm took too much time to teach, and most students simply memorized the algorithm, without grasping the underlying concept. However the 1–5 Rule is quite teachable.

Chem. 104 students also learn that an exact number can never be a least precise factor, because an exact number has infinite precision. From our experience at Oregon State University, we feel that both the 1–5 Rule and the exact number convention are worthwhile and realistic learning objectives for lower division college science courses.

It may also be a good idea to remind students not to throw away information in the middle of a multi-step calculation, by overzealous rounding. Even if one is pressed for time, he or she should always retain <u>at least</u> two more significant figures in an intermediate result than in the least precise factor.

Unlike the 1-5 Rule, the Three Rule demands that students develop a certain level of mathematical maturity. This means that the Three Rule should have greater educational value than the 1-5 Rule, but that it may be less teachable. Therefore the Three Rule may be appropriate for more advanced courses, like physical chemistry.

The Three Rule may be more teachable than the Root Rule Algorithm because its syntax is simpler, because the magic number is simpler, and because its logic is more obvious. However the Three Rule has not yet been tested in the college science classroom.

### Part I Summary and Conclusions

Since significant figure rules depend on propagation of uncertainty, we must define what we mean by "uncertainty". The most reasonable approach is to define uncertainty as the standard error of the mean.

We have presented several new rules for significant figures, in the attempt to avoid the Scylla of invalid generalization (the **Simple Rule**) and the Charybdis of ambiguity (the **Textbook Rule**). The basis for all of the new procedures is the **Root Rule**. The **Root Rule Algorithm** is a computer's eye view of significant figures, which allows the neophyte the opportunity to gain practice in applying the LPF Root Rule correctly, in order to master the underlying concept. This algorithm is the mathematical equivalent of training wheels on a bicycle. The **1–7 Rule** is a preliminary result applied in developing the 1–5 Rule, and is not useful out of this context. Although the **1–5 Rule** (the 'quick and dirty' approach) and the **Three Rule** (which places the most emphasis on propagation of uncertainty) follow from the Root Rule, they are easier to use and may have greater educational value than the parent rule.

The fundamental idea behind any valid significant figure rule is that the percent uncertainty of the product (or quotient) will approximate that of the least precise factor in a calculation. Therefore the number of significant figures used to express the product must imply an uncertainty, which is as close as possible to that implied by the least precise factor.

Algorithms based upon the Root Rule are an alternative to the oversimplified significant figure rule, generally taught in freshman chemistry and physics. The disadvantage of the Root Rule Algorithm is its complexity. The Three Rule is simpler than the Root Rule, and it offers greater insight into the mechanics of propagation of uncertainty. However it has not been tested in the college science classroom.

The 1-5 Rule is more facile than the Three Rule. Since the 1-5 Rule has a simpler syntax and is easier to memorize than the Three Rule, it may also be more teachable. However the Three Rule is more comprehensive. Moreover the Three Rule has greater heuristic value.

Experience has shown that it is practical to teach the 1–5 Rule in General Chemistry courses. Perhaps the Three Rule would be more appropriate for courses at a higher level (eg. physical chemistry). Table 1 summarizes the relative merits of the Simple Rule and the three major new rules for significant figures in multiplication and division calculations.

Table I. A Comparison of the Significant Figure Rules.						
	Correct and comprehensive	Easy to apply, to remember, and to teach	Facilitates understanding of underlying principle			
Root Rule	***	×	***			
Three Rule	***	××	****			
1-5 Rule	**	***	××			
Simple Rule	*	****	×			

In Part II, we will see that it is possible to articulate a more comprehensive rule, which will integrate significant figure theory with simple propagation of uncertainty for the general case of functions of n real variables, each of which contributes appreciable uncertainty.

# PART II: SIGNIFICANT FIGURES AND SIMPLE UNCERTAINTY PROPAGATION THEORY

### The Extended Root Rule

In Part I, we considered the LPF Root Rule as a refinement of the Simple Rule for significant figures. Both rules are quite limited in scope. They apply only to multiplication and division calculations in which

- (a) a single least precise factor (LPF) exists and can be identified
- (b) the least precise factor contributes essentially all of the uncertainty to a product or quotient
- (c) the standard error of the mean definition of uncertainty is used.

It would be desirable to have a more comprehensive significant figure rule.

In the general case, it is necessary to arrive at an **estimated relative uncertainty** of the calculated result, before assigning significant figures. Unless political considerations dictate otherwise, one may use the following rule.

### The Extended Root Rule:

When the result of a calculation is properly rounded, its estimated relative uncertainty to implied relative uncertainty ratio must be between  $1/\sqrt{10}$  and  $\sqrt{10}$  (except when this would mandate a result with less than one significant figure).

The estimated relative uncertainty can be calculated using two different propagation-of-uncertainty formulas, one for each of the two definitions of uncertainty (from Part I). Equation II.1 is for the absolute limit of error type of uncertainty. Equation II.2 is for the standard error of the mean type of uncertainty (which we will emphasize).

$$ERU = \frac{\Delta f}{f} = - \cdot \sum_{i=1}^{n} \cdot \Delta x_{i} + RUM \qquad (11.1)$$
  
f f i=1 dx<sub>i</sub>

$$ERU = \frac{\Delta f}{f} = \frac{1}{f} \left[ \sum_{i=1}^{n} \left\{ \frac{df}{dx_i} \cdot \Delta x_i \right\}^2 \right]^{1/2}$$
(11.2)

where the  $\mathbf{x}_i$  in 11.2 are the measured values of n <u>mutually independent</u> quantities, the  $\Delta \mathbf{x}_i$  are the absolute values of the implied uncertainties of the  $\mathbf{x}_i$ ,  $\mathbf{f}$  is a function of the  $\mathbf{x}_i$ ,  $\Delta \mathbf{f}$  is the absolute value of the uncertainty of f, and  $\Delta \mathbf{f}/\mathbf{f}$  is the absolute value of the estimated relative uncertainty. **RUM** is the maximum relative uncertainty of the method. In a purely theoretical example—such as the area of a perfect rectangle—we may not need to concern ourselves with this. However in some practical applications—like real gas behavior—the calculation method is an approximation, and is itself a source of error. Since the standard error of the mean is really a standard deviation, Equation 11.2 boils down to additivity of variance. In using both equations we must assume that the  $\Delta x_i$  are all reasonably small (which is not always true, especially for  $x_i$  which have only one significant figure).

If the components of a physical calculation are represented by stand-alone significant figures, then the Extended Root Rule and Equation II.2 will allow us to express the result in the same way. Moreover the uncertainties of any of the calculation's components and of the calculation's result can always be pinned down within a ten-fold range.

A consequence of the Extended Root Rule and of Equation II.2, is that at least one significant digit will be lost for **homogeneous addition** calculations in which 10 or more quantities are summed. Consider the following addition calculation: 12.3 57.1 11.3 17.1 92.3 29.3 13.7 41.4 34.7 <u>53.5</u> <u>3</u>62.7

Since we are adding 10 quantities, all of which have appreciable uncertainty in the tenths' place (hence the homogeneity), the sum should be rounded to 363. Here we are assuming that the uncertainty in the tenths' place is the same for each quantity. If we insist on using the absolute limit of error type of uncertainty with homogeneous addition, then we will lose a significant figure when there are four or more terms!

As another example, let's suppose that x = 1.111 and that  $f(x) = \log (x) = 0.045714$ . By Equation 11.2,

 $\frac{\Delta f}{-} = \frac{df}{-} \cdot \frac{\Delta x}{-} = \frac{\log e}{-} \cdot \frac{\Delta x}{\Delta x} = \frac{0.001 * \log e}{-} = 0.00855$ f dx f x log x 1.111 \* 0.045714

Therefore when correctly rounded, the logarithm is 0.046, since

$$\frac{0.001/0.0457}{0.00855} = 2.56 < \sqrt{10}$$

Note that two significant figures were lost.

As another example, let's apply the Extended Root Rule to a gas chromatography calculation. The affinity of a particular compound for a given stationary phase is commonly expressed in terms of the **retention index I** which can be calculated as follows (writing "In"

instead of the conventional base 10 log for mathematical simplicity, since it makes no difference in the resulting value of 1):

$$I = 200 * \frac{\ln x - \ln t_6}{\ln t_8 - \ln t_6} + 600$$

where  $t_6$  and  $t_8$  are the sorbed times of n-hexane and n-octane, which happen to precede and to follow the sample peak, whose sorbed time is x. The numerical values of  $t_6$ , x, and  $t_8$  are 10.5, 18.8, and 53.0, respectively. The units are "mm of chart paper". Converting these units to units of seconds or minutes will not affect the value of I.

$$\frac{dI}{dt_{6}} = 200 * \frac{I(\ln t_{8} - \ln_{6}) - (\ln x - \ln t_{6})I * (-1/t_{6})}{(\ln t_{8} - \ln t_{6})^{2}}$$

$$= \frac{200 * (\ln x - \ln t_{8})}{t_{6} * (\ln t_{8} - \ln t_{6})^{2}} = \frac{200 * (\ln 18.8 - \ln 53)}{10.5 * (\ln 53 - \ln 10.5)^{2}} = -7.532$$

$$\frac{dI}{dx} = \frac{200}{x * (\ln t_{8} - \ln t_{6})} = \frac{200}{18.8 * (\ln 53 \ln 10.5)} = 6.571$$

$$\frac{dI}{t_{8}} = \frac{-200 * (\ln x - \ln t_{6})}{t_{8} * (\ln t_{8} - \ln t_{6})} = \frac{-200 * (\ln 18.8 - \ln 10.5)}{53 * (\ln 53 - \ln 10.5)} = -0.839$$

Without loss of generality, we will use a ±1 convention for all of the above variables. (A different  $\pm$  convention would not have a great effect on the significant figure determination.) Thus  $\Delta t_6 = \Delta x = \Delta t_8 = 0.1$  By Equation 11.2,

ta

$$\frac{\Delta f}{f} = \frac{\Delta t}{f} * \left[ \left\{ \frac{dI}{dt_6} \right\}^2 + \left\{ \frac{dI}{dx} \right\}^2 + \left\{ \frac{dI}{dt_8} \right\}^2 \right]^{1/2}$$
$$= \frac{0.1 * \left[ (-7.532)^2 + 6.571^2 + (-0.839)^2 \right]^{1/2}}{671.96} = 0.001493$$

This is the estimated relative uncertainty. The next step is concerned with the implied relative uncertainty. We need to determine the number of significant figures necessary to minimize the discrepancy between the values of the implied relative uncertainty and of the estimated relative uncertainty (**ERU**). It turns out that the properly rounded answer is 672 (three significant figures). The implied relative uncertainty (**IRU**) of 672 is 1/672 = 0.001488. Then

$$\frac{\text{ERU}}{\text{IRU}} = \frac{0.001493}{0.001488} = 1.04 < \sqrt{10}$$

and the Extended Root Rule is satisfied.

In Part I we showed that the LPF Root Rule was relatively independent of  $\pm$  convention. The same applies to the Extended Root Rule. The purpose of this rather arcane section is to deal with those few cases where we do have to worry about the  $\pm$  convention. Our frame of reference will be the standard error of the mean definition of uncertainty.

The Extended Root Rule applies when not all of the numerical values of the uncertainties  $(\Delta x_i)$  are available. If the numerical values for <u>all</u> of the  $\Delta x_i$  are given, then what is the point in being limited to standalone significant figures? As in Part I, we assume that the same ± (hindsight) convention applies for estimating the unknown uncertainties of the  $x_i$ . We are free to choose any reasonable ± convention. Usually a ±1 convention is easiest to work with. For ordinary significant figure determinations, our results are not usually affected by this choice. However the ± convention is relevant for **mixed significant figure determinations**, in which some—but not all—of the components' estimated uncertainties are available.

Thus far, we have approached significant figures from a **hindsight** perspective. The experimenter deposits information about estimated uncertainty within the number of significant figures of a measurement-based quantity. Then we see the number, and interpret it in <u>hindsight</u>, inferring some uncertainty not specified by the experimenter. In the multiplication and division calculations of Part I, our task has been to transfer this inferred uncertainty from the least precise factor (LPF) to the product or quotient.

Now we will ask a new kind of question. What is the most reasonable hindsight (±) convention? Our answer will depend upon which rounding convention we choose, that is how much uncertainty is allowed in the last significant digit of the data being manipulated.

We will choose the most generous rounding convention allowed by he Mainstream approach. The maximum uncertainty we will allow on the last significant digit of a measurement-based quantity is ±5. Consider the following example:

9.23 ± 0.06

The absolute value of the uncertainty (6) on the tentative last significant digit (on the "3") is greater than 5. Therefore the "3" should be rounded off, leaving only two significant figures.

9.23 ± 0.06 → 9.2

If an experimenter follows the custom that estimated uncertainties greater than ±5 on any digit will be eliminated by rounding off that digit, then we may infer that the last reported digit has an estimated uncertainty no greater than ±5, and no less than ±0.5. (Obviously the upper uncertainty limit does not always apply to the anomalous one-significant-figure-quantities.) We have no way of knowing from the reported datum what the estimated uncertainty really was, except that it was between these limits. Since the limits are an order of magnitude apart, we will argue from the same logic that led to the Root Rule, that the best guess of the estimated uncertainty on the last digit will be half an order of magnitude into the range, or  $\pm 5/\sqrt{10} = \pm 1.58$ .

Now we'll take an indirct route back to the hindsight conventions we have just described. We will use the following borderline case of the LPF Root Rule to pin down some uncertainties:

Our argument will hinge upon the common-sense notion that if a calculation is borderline with respect to the LPF Root Rule, then it should also be borderline with respect to the most reasonable hindsight convention. Let A and B be the expected\* uncertainties on the last digit of the least precise factor, and of the tentative last significant digit of the quotient, respectively. Then

$$\frac{A}{2.65} = \frac{B}{8.38} \qquad B = \frac{8.38}{2.65} * A \approx A \sqrt{10} \qquad A \approx \frac{B}{\sqrt{10}}$$

<sup>&</sup>quot;In this argument, we are not using "expected" in its mathematical sense; here "expected" refers to the median, rather than the mean.

Notice that in this borderline case the least precise factor and quotient mantissas differ by a factor of approximately  $\sqrt{10}$ . Since this is near the maximum allowed by the LPF Root Rule, it suggests that the uncertainty on the tentative last significant digit of the quotient has been stretched to the allowable maximum. Thus we would expect the uncertainty on the final "8" (in the quantity "8.38") to be approximately  $\pm 5$ . (We would not expect this uncertainty to be  $\pm 6$  or  $\pm 4$ , because then the quotient would <u>definitely</u> have two significant figures, or three significant figures, respectively.) Thus

 $A = 5/\sqrt{10} = 1.58$ 

For our  $\pm 0.5$  to  $\pm 5$  rounding convention, the most reasonable hindsight convention is approximately  $\pm 1.58$ . Note that 1.58 is the geometric mean of 0.5 and 5. In general, the hindsight convention value is approximately equal to the geometric mean of the rounding convention limits.

In a mixed significant figure determination, where only some of the components' estimated uncertainties are known, the ideal procedure should be as follows:

- Apply the hindsight (±) convention value to the last significant digit of any calculation component, whose estimated uncertainty is not known.
- Plug these values, together with the given estimated uncertainties, into Equation II.2.
- 3) Then proceed as before, using the Extended Root Rule.

In the absence of standardized rounding and hindsight conventions, this variation on our basic theme is not yet possible. However the hindsight convention concept has broader implications. In this discussion, we have ignored the effect of rounding error, a situation which we now will remedy.

The reporting of a measurement-based quantity involves the following three types of error:

- 1) Random error.
- 2) Systematic error.

3) **Rounding error**. An example of a pure rounding error is that which arises when  $\pi$  is rounded to 3.14 (or to 3.141592654 for that matter). The very fact of rounding introduces an error, and sometimes this must be taken into consideration. Rounding error must be distinguished from **measurement error**, which includes (1) and (2) above.

According to Sheppard<sup>4</sup>, the variance of a rounded variable equals the variance of the unrounded variable plus R<sup>2</sup>/3, where ±R are the rounding error limits. Recall that the ±1.58 hindsight convention (associated with the ±5 rounding convention) refers to measurement uncertainty only. The corresponding **total uncertainty hindsight convention** would be estimated as follows (remembering that 1.58 is an approximation of  $5/\sqrt{10} = \sqrt{2.5}$ ):

$$\pm\sqrt{2.5 \pm 0.5^2/3} = \pm 1.61$$

which is not very far from ±1.58.

At this point, we have three choices. First we could amend (and complicate) the Root Rule in order to take rounding error into account. Secondly we could continue to ignore the effect of rounding error. Lastly, we could retain the Root Rule, and multiply the right hand side of Equation 11.2 by a correction factor. In this case, the correction factor would be calculated as follows:

$$F_{1.58} = \left[\frac{2.5 + 1/12}{2.5}\right]^{1/2} = \left[\frac{31}{30}\right]^{1/2} = 1.0165$$

It must be understood that the rounding error correction factor is a function of the hindsight convention (for measurement uncertainty). For example, if our hindsight convention is  $\pm 1$  (which goes along with  $\pm 1/\sqrt{10}$  to  $\pm\sqrt{10}$  rounding convention limits), then this correction factor would be calculated as follows:

$$F_1 = \left[\frac{1^2 + 1^2/12}{1^2}\right]^{1/2} = \left[\frac{13}{12}\right]^{1/2} = 1.0408$$

Our main purpose in exhuming rounding error is to show that it is relatively inconsequential for ordinary significant figure determinations involving the standard error of the mean type of uncertainty. However rounding uncertainty would be relatively important for mixed determinations in which any of the uncertainties given are substantially less than the  $\pm 1.58$  hindsight convention would suggest. Since the above correction factor (F) increases as the hindsight ( $\pm$ ) convention decreases, rounding uncertainty <u>must</u> be taken into account if the absolute value of the hindsight convention is substantially less than unity.

For significant figure determinations which use the absolute limit of error type of uncertainty, the total uncertainty hindsight convention is

 $\pm(1.58 \pm 0.5) = \pm 2.08$ 

Therefore the LPF Root Rule would have a decidedly optimistic bias if the absolute limit of error type of uncertainty was employed, unless the Liberal approach was used also. (See Part I.)

In this section, we have seen how the concept of rounding convention leads to that of hindsight convention, which should be taken into account during mixed significant figure determinations. We also considered rounding error, and its effects on the total uncertainty hindsight convention <u>vis-a-vis</u> the absolute limit of error and standard error of the mean definitions of uncertainty (See Part I). All of these considerations underscore the importance of establishing a standardized rounding convention.

#### Part II Summary and Conclusion

We have seen that the Root Rule is a rational basis for significant figure determinations. The Extended Root Rule says that we must compare the estimated relative uncertainty and implied relative uncertainty for the rounded numerical result R of a chemical or physical calculation. The estimated relative uncertainty and implied relative uncertainty of R must be in the same ballpark, i.e. within half an order of magnitude of each other. If they are, then R has been rounded to the correct number of significant figures.

In Part II, we saw that the value of the estimated relative uncertainty we obtain depends on which definition of uncertainty we use. This needs to be standardized.

In Part I, we considered only the special case where the estimated relative uncertainty of a product or quotient is approximately equal to the implied relative uncertainty of the least precise factor for a multiplication or division calculation, in which the standard error of the mean definition of uncertainty is used. This leads to the LPF Root Rule (and to the handy 1–5 Rule). Thus the LPF Root Rule of Part I is a special case of the Extended Root Rule.

All of these procedures can be incorporated into computer programs. Some calculators (eg. the Hewlett-Packard 15C) allow the user to choose in advance the number of significant figures which will appear in the display. Perhaps scientific calculators of the future will have the capability of doing significant figure determinations. This raises the possibility of eliminating extraneous-digit noise from modern electronic calculators (and from freshman chemistry lab reports).

# APPENDIX

First we will show that the LPF Root Rule and the Simple Rule give different results more than 18% of the time in two-factor multiplication calculations. We will make the following assumptions:

- (a) All (base 10) mantissas are equally likely.
- (b) The two factors do <u>not</u> have the same number of significant figures.

This second assumption is reasonable. If both factors have the same number of significant figures, then it is not true that the LPF contributes essentially all of the uncertainty. Therefore by hypothesis, neither the Simple Rule nor the LPF Root Rule should be used. Moreover we will ignore the problems created by the anomalous one-significant-figure-quantities.

Let  $M_1$  and  $M_2$  be the smaller and larger mantissas of the two factors. The LPF can override the Simple Rule only when the following conditions are both met:

1) 
$$M_1 < \sqrt{10}$$

2)  $M_2 > \sqrt{10}$ 

Suppose that Conditions 1 and 2 are true. Then we have the following cases and subcases to consider:

- I. The product mantissa is less than  $\sqrt{10}$ .
- II. The product mantissa is greater than  $\sqrt{10}$ .
- A. The LPF mantissa is less than  $\sqrt{10}$ .
- B. The LPF mantissa is greater than  $\sqrt{10}$ .

There will be an override (of the Simple Rule) if and only if either IB or IIA is true. In Equations A.1-3, we will assume that Conditions 1 and 2 (above) are true. Therefore the probabilities (represented by P) in these equations are <u>conditional</u>. By Conditions 1 and 2,

$$P(IA) = P(IB)$$
 and  $P(IIA) = P(IIB)$  (A.1-2)

$$P(IB) + P(IIA) = P(IA) + P(IIB)$$
 (A.3)

Thus the <u>conditional</u> probability  $(P_1)$  of an override, given (1) and (2), is exactly 0.5.

The probability that Conditions 1 and 2 are both true is given by the following:

$$P_2 = \frac{\sqrt{10} - 1}{10 - 1} \cdot \frac{10 - \sqrt{10}}{10 - 1} \cdot 2$$
 (A.4)

Therefore the <u>unconditional</u> override probability is given by the following:

$$P = P_1 P_2 = 0.5 \cdot \frac{\sqrt{10} - 1}{9} \cdot \frac{10 - \sqrt{10}}{9} \cdot 2 = 18.3\%$$
 (A.5)

In division calculations, the LPF Root Rule will override the Simple Rule nearly 30% of the time. Here, we need to consider the following cases and subcases:

- I' The least precise factor is in the numerator.
- A' The quotient mantissa (Q) is less than the least precise factor mantissa (L).
- B' Q > L

Therefore

II' The least precise factor is in the denominator.

<u>Case IA</u>' Suppose that the least precise factor is in the numerator. Let M be the mantissa of the most precise factor. Let P(IA') be the probability of a IA' division override. Override will occur if and only if  $\sqrt{10} \le M \le L$ . Therefore

$$P(1A') = 0.5 \left[ \frac{10 - \sqrt{10}}{10 - 1} \right]^2 = 5 \left[ \frac{\sqrt{10} - 1}{9} \right]^2$$
(A.6)

<u>Case IB</u>' Override will occur if and only if  $L < M < \sqrt{10}$ . Therefore

$$P(IB') = 0.5 \left[ \frac{\sqrt{10} - 1}{10 - 1} \right]^2$$
(A.7)

$$P(I') = P(IA') + P(IB') = 5.5 \left[\frac{\sqrt{10} - 1}{9}\right]^2$$
 (A.8)

Case II' is somewhat more complicated. Let x be the denominator mantissa. We must consider the following four subcases:

1)  $1 \le x \le 10^{.25}$ 2)  $10^{.25} \le x \le \sqrt{10}$ 3)  $\sqrt{10} \le x \le 10^{.75}$ 4)  $10^{.75} \le x \le 10$ 

Let  $\overline{P}_i$  be the probability that subcase i applies. The  $\overline{P}_i$  are calculated as follows:

$$\overline{P}_{1}' = \frac{10^{-25} - 1}{10 - 1} = 0.08647549$$
(A.9)

$$\overline{P}_{2}' = \frac{\sqrt{10} - 10^{.25}}{10 - 1} = 0.1537775833$$
(A.10)

$$\overline{P_3}' = \frac{10^{.75} - \sqrt{10}}{10 - 1} = 0.2734595102$$
 (A.11)

$$\overline{P_4}' = \frac{10 - 10^{.75}}{10 - 1} = 0.4862874164$$
(A.12)

Let  $P_i$  be the conditional probability that there will be an override, given that subcase i applies.

In subcase 1, override will not occur if and only if the numerator mantissa is between x and  $x^2\sqrt{10}$ . If x is fixed, then

$$1 - P_1'(x) = \frac{x^2 \sqrt{10} - x}{10 - 1}$$
(A.13)

The subcase 1 frequency function is as follows:

$$f_1(x) = 1/(10^{-25} - 1)$$
 (A.14)

Therefore the average (expected) value  $P_1$  of  $P_1(x)$  is calculated as follows:

$$P_{1}' = 1 - \int_{1}^{10^{-25}} P_{1}'(x)f_{1}(x)dx = \int_{1}^{10^{-25}} \frac{x^{2}\sqrt{10} - x}{9(10^{-25} - 1)} dx$$
  
= 0.458581526 (A.15)

The subcase 2 calculations are as follows:

$$P_{2}'(x) = \frac{x - x^{2}/\sqrt{10}}{10 - 1} \qquad f_{2}(x) = \frac{1}{\sqrt{10} - 10^{-25}} \qquad (A.16-17)$$

$$P_{2}' = \int_{10^{-25}} P_{2}'(x) f_{2}(x) dx = \int_{10^{-25}} \frac{x - x^{2}/\sqrt{10}}{9(\sqrt{10} - 10^{-25})} dx$$

$$= 0.05445476057 \qquad (A.18)$$

The subcase 3 calculations are as follows:

$$P_{3}'(x) = \frac{x^{2}/\sqrt{10} - x}{10 - 1} \qquad f_{3}(x) = \frac{1}{10^{.75} - \sqrt{10}} \qquad (A.19-20)$$

$$P_{3}' = \int_{\sqrt{10}}^{10.75} P_{3}'(x) f_{3} dx = \int_{\sqrt{10}}^{10.75} \frac{x^{2}/\sqrt{10} - x}{9(10^{.75} - \sqrt{10})} dx$$

$$= 0.206723907 \qquad (A.21)$$

The subcase 4 calculations are as follows:

$$P_{4}'(x) = \frac{x - x^{2}/\sqrt{1000}}{10 - 1} \qquad f_{4}(x) = \frac{1}{10 - 10^{.75}} \qquad (A.22-23)$$

$$P_{4}' = \int_{10.75}^{10} P_{4}'(x) f_{4}(x) dx = 1 - \int_{10.75}^{10} \frac{x - x^{2}/\sqrt{1000}}{9} dx$$

$$= 0.3520532293 \qquad (A.24)$$

The override probability (given that the least precise factor is in the denominator) is calculated as follows:

$$P'(11) = \sum_{i=1}^{4} \overline{P_i} P_i = 0.2760191157$$
 (A.25)

If we assume that the least precise factor will end up in the numerator as often as in the denominator, then the unconditional override probability (P') for division calculations is given by the following:

$$P'= 0.5 [P'(1) + P'(11)] = 29.7\%$$
 (A.26)

If we assume that division and multiplication are equally frequent, then the overall override probability would be about 24%, since 24% is the average of 18.3% (for multiplication) and 29.7% (for division).

In the above arguments, we have assumed that the mantissa frequency function f is a constant (1/9 in the unrestricted case). A more realistic approach would set f = c/x, where x is the mantissa, and c is a constant (c = 1/ln 10 in the unrestricted case). A similar argument, using this second assumption leads to the result that

$$P = P'(I) = P'(II) = 25\%$$
 exactly (A.27)

Thus the Simple Rule not only breaks down, but it does so with embarrassing frequency.

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# DECIMAL CODED BINARIES: A TECHNIQUE FOR COMPRESSING A MEASUREMENT AND ITS UNCERTAINTY INTO A SINGLE QUANTITY

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#### ABSTRACT

The theoretical and applied aspects of Decimal Coded Binaries, a new method for compacting scientific data into a tabular format, are explored. This technique efficiently combines a measurement and its uncertainty into a single easy-to-read quantity. DCB compares favorably with a pedestrian reference technique for accomplishing the same end (and with ordinary stand-alone significant figures). The DCB algorithm has been programmed into a hand-held scientific calculator, and into a simple microcomputer which is used as an interface with chemical instruments commonly utilized in quantitative analysis.

#### INTRODUCTION

Suppose that you are giving complicated street directions, and that the other person's attention seems to be flagging. Unconsciously you may raise the pitch of your voice for the last word of a sentence. ("And then you turn <u>left</u>.") A casual eavesdropper will understand the "turn left", but may jump to the conclusion that you are asking a question, when in fact your tone of voice is a polite way of saying, "Listen to me!" Of course, the intonation change in the word "left" will require a little extra time because the vowel is drawn out slightly, but less time than it would take to say, "Listen to me!" Thus the use of inflection can enhance the efficiency of communication. In the above parable the way we end the "turn left" sentence has an indirect meaning, above and beyond the meaning of the words themselves.

We will describe a new method for compressing scientific data— Decimal Coded Binaries, or DCB, and an auxiliary technique, Linear Code. Like the sentence in the parable, a quantity which has been coded by either technique will have both a direct and an indirect meaning.

The direct meaning is the number itself, which is approximately equal to the value of the measurement. The "indirect meaning" is the information about the measurement's uncertainty, which we will infer from the last digit of a Linear Coded quantity, and from the last several <u>binary</u> digits of a DCB quantity. Like the sentence in the parable, DCB is efficient. DCB requires appreciably less space on paper or in memory devices, and less time for telecommunicating than would be required to write, store, or transmit the value of the measurement and its uncertainty separately. Both techniques are user-friendly in the sense that it is easy to program coding and decoding routines into ordinary microcomputers and HP15C calculators. Before we describe these coding techniques, we will discuss the reporting of measurement-based data.

There is a consensus among physical scientists that when a measurement is reported, some indication of its trustworthiness should also be given. There are two widely-used methods for expressing the trustworthiness of a measurement.

In the direct approach, the experimenter gives a full accounting of the measurement and its limitations. He or she will report how reproducible the results are and also discuss what is known or surmised about the systematic error. NBS Handbook 91<sup>5</sup> gives a very comprehensive treatment of the direct approach. However this scientific prescription for description is honored more in the breach than in the observance.

Sometimes it is impractical to be this explicit, especially in data tables. When brevity and readability are the chief concerns, standalone significant figures are often used instead of the direct approach, but there are serious problems associated with this usage of significant figures.

Significant figures are a sacred cow in the sense that most scientists can agree about the sacredness, but few can agree on the nature of the cow! Almost every physical scientist has a strong opinion about significant figures, and regards his or her interpretation as being obviously correct. However there are truly fundamental differences of interpretation to be found in the literature.

The current NBS usage<sup>6</sup> of stand-alone significant figures is quite narrow. There is an upper bound on the maximum relative uncertainty allowed on the last reported digit of a measured quantity, but there is no lower bound. Here the last reported (significant) digit must be known with certainty; i.e. the estimated uncertainty on the last reported digit must not exceed  $\pm 0.5$ . (We will attempt to define uncertainty shortly.) In an extreme case, a mass measurement of 123.4 mg, with an estimated uncertainty of 0.6 mg, would have to be reported as  $1.2 \times 10^{1}$  mg since the third digit could be "3" or "4". In the following example, we will consider the question: What is the proper number of significant figures that should be used to write the atomic weight of aluminum, according to the NBS?

The atomic weight of aluminum is

- (a) 27, correct to two significant figures.
- (b) 27.0, correct to three significant figures.
- (c) 26.98, correct to four significant figures.

According to the NBS, all of the above are syntactically correct. Therefore there is no <u>unique</u> answer to the question we have just posed. In the NBS Weltanschauung, significant figures are not supposed to give very much information about the uncertainty of a measurement.

Skoog and West<sup>7</sup> take a broader approach, in which stand-alone significant figures are used to give more information about the estimated uncertainty. Here the estimated uncertainty on the last significant (reported) digit must be between  $\pm 0.5$  and  $\pm 5$ . Using this  $\pm 0.5$  to  $\pm 5$  rounding convention, the mass measurement example would be rounded to 123 mg. The "3" in "123" has meaning even though it is not known with certainty.

In this general approach, the reader of the data can infer that the estimated uncertainty must be within a particular ten-fold range (which is not to be confused with a confidence interval). This is not true for the narrow NBS approach.

A second problem is that there is a lack of consensus on the meaning of uncertainty. Let's review some fundamentals.

There are two sources of measurement error: **random error** (sometimes called imprecision) and **systematic error** (sometimes called determinate error). Random error occurs when repeated measurements of the same thing yield somewhat different values. The smaller the random error, the greater the precision. A measurement will be relatively accurate if both random and systematic errors are small.

Skoog and West have suggested that systematic (determinate) errors may be classified with respect to their sources and their effects. "It is not possible to list all conceivable sources of determinate error; we can, however, recognize that they have their origin in the <u>personal</u> errors of the experimenter, the <u>instrumental</u> errors of his measuring devices, the errors that repose in the <u>method</u> of analysis he employs, or any combination of these."<sup>8</sup>

"Determinate errors generally fall into either of two categories, <u>constant</u> or <u>proportional</u>. The magnitude of a constant error is independent of the size of the quantity measured. On the other hand, proportional errors depend in absolute magnitude upon, and increase or decrease in proportion to, the size of the sample taken for analysis."<sup>9</sup>

We will add a third classification scheme. All systematic errors come under one of the following two categories:

- 1) <u>suspected</u> systematic errors
- those we are completely unaware of, i.e. <u>lurking</u> systematic errors. By definition, lurking systematic errors cannot be compensated for, or taken into account.

**Uncertainty** is a key concept in this discussion. Both random error and systematic error can undermine our sense of certainty in a measurement, but what does uncertainty really mean? Unfortunately, a direct answer to such a philosophical question is beyond the scope of this paper. However we can approach the question in a pragmatic fashion. What kind of uncertainty is most useful to us? We will compare four types (definitions) of uncertainty.

 The first type of uncertainty is the <u>absolute limit of error</u> in a measurement. The advantages of using this kind of uncertainty are that both random error and suspected systematic error are included, and that the simple worst case method<sup>10</sup> of error analysis can be used to trace the propagation of uncertainty in a calculation. By definition, lurking systematic error cannot be taken into account; hence the "absolute limit of error" of a measurement is unknown and unknowable. Moreover if the random error is normally distributed, as we so often assume, then these limits don't even exist, since the Gaussian frequency function will yield a non-zero probability density for any real value of the random variable. In an extreme case, this means that there is a non-zero (albeit very small) probability that any truly normal random variable will be 10 million standard deviations away from the mean of the distribution.

- 2) The second type of uncertainty we will consider is the maximum <u>suspected</u> systematic error. Unlike (1) above, this kind of uncertainty could apply to the real world. If the suspected systematic error is large, relative to the imprecision, then the reader of the data would like to know about it. However it would be difficult to reduce even the <u>suspected</u> systematic error to a single number. If the suspected systematic error is mentioned at all when a measurement is reported, the experimenter will usually attempt is to discuss it thoroughly. The next two classes of uncertainty are functions of the imprecision.
- 3) Our index of uncertainty could be one half of a 95% confidence interval, the **half-span**. However there are two limitations:
  - (a) Systematic error cannot be taken into account, since this kind of uncertainty applies only to random error.
  - (b) Confidence intervals do not lend themselves to propagation-ofuncertainty analysis. (See Appendix.)
- 4) The standard error of the mean is a better way of expressing the uncertainty stemming from imprecision. This definition, like the preceding one, applies only to random error, and not to systematic error. However propagation-of-uncertainty analysis is relatively simple under this definition (unlike Definition 3); it applies to the real world (unlike Definition 1); and the standard error of the mean can be written quite compactly (unlike a suspected systematic error, which may require several paragraphs of explanation and caveats).

Our primary objective in developing these data compression techniques is to provide a compact format, which will enable the experimenter to report a measurement, together with an index of its trustworthiness. If neither the random error nor the suspected systematic error are negligible, then both types of error limit the trustworthiness of the measurement. A satisfactory definition of uncertainty must make sense and it should take both types of error into account.

None of the above definitions are fully adequate, although (4) is the most reasonable, and it is this standard error of the mean definition that we will emphasize. We will denote this type of uncertainty by **Um**, an abbreviation for the **estimated uncertainty of the measurement**.

Now that we have exhausted uncertainty definitions, we must consider one final problem with stand-alone significant figures, as they are ordinarily used. Even with the general approach of Skoog and West (which we will use in modified form), the estimated uncertainty on the last significant digit of a measurement-based quantity can be anywhere within a ten-fold range (because of the base ten number system). In the next two sections, we will describe two types of data compression techniques, which address this problem. In order to make Decimal Coded Binaries (DCB) more understandable, we will develop an auxiliary technique in the next section. DCB will be introduced in the section after that.

#### LINEAR CODE

Now we will return to the linguistic parable introduced in the previous section, where we had briefly discussed inflection, a commonly-used speech compression technique. Clearly this is not the only way to condense communications. The obvious approach is first to use abbreviations whenever possible, then to eliminate the non-essential words (eg. articles), then finally to delete the periods at the ends of sentences and the spaces between words. We will contemplate how such a sequence of compaction steps could apply to quantitative data. Then we will see how Linear Code puts this Western Union approach into practice.

As a first step, we could decide how many digits to report for a measured value. (How many significant figures does the quantity have?) Then we would round off the number accordingly.

Secondly, we could use a one-digit code to indicate the imprecision on the last reported digit of the measured value. This **uncertainty code** would give the reader of the data the upper and lower bounds for the estimated standard error of the mean.

The last steps in this pedestrian data compaction technique would be to condense the format for reporting the uncertainty code. Instead of writing "standard error of the mean = " or "±", we could simply leave a space between the measured value and the uncertainty. Finally we could delete even the above space, by tacking the uncertainty code onto the end of the **mantissa** of the number representing the measured value. (Suppose that a number expressed in scientific notation is  $3.16 \times 10^{-2}$ . The "3.16" is called the mantissa.)

Now let's talk about the actual technique. The following two steps summarize the procedure for expressing a measurement in Linear Code:

- 1. Round the value of the measurement-based quantity to the correct number of significant figures, using scientific notation if necessary.
- Insert a digit after the last significant figure. This extra digit is the uncertainty code, and it has nothing to do with the measurement's value.

Table II illustrates the uncertainty code concept, as tentatively applied to the  $\pm 0.5$  to  $\pm 5$  rounding convention of the previous section.

Table IIRelationship Between Uncertainty Code and Estimated Measurement Uncertainty with the ±0.5 to ±5 Rounding Convention.				
Uncertainty Code				
0 1	2 3 4 5 6 7 8 9 1 1.3 1.6 2 2.5 3.2 4 5			
Estimated measurement uncertainty				

Note that Table I uses a semilogarithmic scale for the bottom row. This allows the estimated measurement uncertainty to be pinned down within a  $10^{0.1}$ -fold range. For instance, if the uncertainty code is 4, then the estimated measurement uncertainty on the last significant digit would be between 1.3 and 1.6. As an example, the Linear-Coded quantity "59.4 ppm" translates into plain English as "59 ppm, with an estimated measurement uncertainty between 1.3 ppm and 1.6 ppm". (This is not the same as a confidence interval.) However there is a fly in the ointment.

Thus far, we have only considered uncertainties which come from measurement errors; **rounding errors** also need to be taken into account. An example of a pure rounding error is that which arises when  $\pi$  is rounded to 3.14 (or to 3.14159265 for that matter). According to Sheppard<sup>11</sup>, the **total standard deviation**  $s_T$  of a reported measurement can be calculated as follows:

$$s_T = (s^2 + R^2/3)^{1/2}$$
 (1)

where s is the standard deviation of the measurement, and R is the maximum possible rounding error (which is ±0.5 on the last significant

digit). Now we will introduce the concepts of rounding ratio and estimated total uncertainty  $U_T$ .

$$U_{\rm T} = (Um^2 + R^2/3)^{1/2}$$
 (3)

where **Um** is the estimated measurement uncertainty, as defined in the previous section. Note that Equations 1 and 3 are isomorphic.

Eisenhart<sup>12</sup> recommends that a quantity be rounded such that the rounding ratio is at least two. This suggestion can be appreciated with the help of the concept of the **%** inflation (of uncertainty).

% inflation = 
$$100(U_T - Um)/Um$$
 (4)

The minimum estimated measurement uncertainty (Um) we have been allowing on the last reported digit is  $\pm 0.5$ . By Equations 3 and 4, this would result in a 15% inflation; i.e. the total estimated uncertainty would be 15% more than the estimated measurement uncertainty. This would be very frustrating for the poor experimenter who has been so diligent in controlling temperature, pressure, humidity, and other extraneous variables, only to have a rounding convention inflate his or her imprecision by 15%! Table III summarizes the relationship between estimated measurement uncertainty (Um), rounding ratio, and inflation.

Table III	Relationship Between Estima Measurement Uncertainty, Rounding Ratio, and Inflation		3		
Um Rounding ratio % inflation	0.5 1 15.47	2	4	3 6 0.46	5 10 0.17

Table IV shows the relationship between uncertainty code and estimated total uncertainty  $(U_T)$  with our current rounding convention (±0.5 to ±5).

Table IVRelationship Between Uncertainty Code and Estimated Total Uncertainty with the ±0.5 to ±5 Rounding Convention.				
Uncertainty code				
<u>  0   1</u> .58 .69	<u>1 2 3 4 5 6 7 8 9 </u> .84 1 1.3 1.6 2 2.5 3.2 4 5			
Estimated total uncertainty				

Now compare Tables I and III. Note the difference between Um and  $U_T$  in the lower uncertainty codes. Our task would be simplified greatly if this discrepancy were minimized. We could accomplish this by changing the rounding convention.

For purposes of Linear Code, we will adopt the convention that the estimated measurement uncertainty (Um) on the last significant digit will be between  $\pm 2$  and  $\pm 20$ , in order to have a reasonably small inflation. The minimum rounding ratio allowed by this rounding convention is calculated as follows:

## min. rounding ratio = 2/0.5 = 4

According to Table III, this corresponds to an inflation of 1.04%, which is tolerable, even by Swiss standards. Thus Table II is merely a trial balloon for a widely-used rounding convention. For the actual application of linear coding (with the  $\pm 2$  to  $\pm 20$  convention), Table V must be used.

Table VRelationship Between Uncertainty Code and Estimated Measurement Uncertainty for the ±2 to ÷20 Rounding Convention.				
Uncertainty code				
<u>  0   1</u> 2 2.5	<u>2 3 4 5 6 7 8 9</u> 3.2 4 5 6.3 8 10 12.6 15.9 20			
Estimated measurement uncertainty				

If we mistake a Linear Coded quantity for an ordinary base 10 number, then we lose out on the uncertainty. But the value of the measurement does not suffer appreciably from the misinterpretation. In the worst case scenario, the misinterpretation error on the last reported digit is 9, as compared with the measurement uncertainty on the last reported digit which is at least 159. Therefore the maximum misinterpretation error is

#### 9/159 ≈ 5.7%

of the uncertainty. So Linear Code is very forgiving to the reader of a data table, who has never heard of Linear Code, and mistakes it for ordinary base 10 notation.

Economy is the primary rationale for using any kind of data compaction technique (or even stand-alone significant figures) in lieu of directly reported uncertainties. Therefore it would be prudent to calculate the cost of Linear Code relative to the ordinary (stand-alone) usage of significant figures.

There are two cost components, the first of which is the one extra digit for the uncertainty code. Therefore Cost 1 = 1 digit. The second component is equal to the probability that a quantity, which has been tentatively rounded in accordance with the ±0.5 to ±5 convention, will need an extra digit in order to satisfy the new ±2 to ±20 convention. This may be calculated as follows:

# Cost 2 = log (2/0.5) = 0.602 digits

Now we will calculate the total relative cost of linear coding.

## Total cost = Cost 1 + Cost 2 = 1 + 0.602 = 1.602 digits

Thus Linear Code is more expensive than stand-alone significant figures. However Linear Code gives much more information about the estimated measurement uncertainty of an experimental parameter. Moreover Linear Code is a very understandable method. Eventually we will see that it is mainly useful as a reference technique. In the next section, we will introduce a data compaction method, which is more efficient than linear code. We will see that this technique also has convenient human engineering features.

#### DECIMAL CODED BINARIES

We will return once again to our linguist parable. We saw that the essence of "Listen to me!" is found in the altered tone of voice, rather than the words themselves. When we combined the meanings of the actual street directions and this auxiliary sentence in a compact form, all we did was to add an upscale glissando to the end of the otherwise monotonic "Then-you-turn-left" in order to create the desired effect (lifting the other person out of his or her lethargy). In this example, the key to efficient data compaction is the ending of the sentence.

As we mentioned earlier, there is a striking parallel between the linguistic parable and our data compression techniques. In the Linear Coding technique of the previous section, we focused on the <u>base 10</u> endings of numbers, which is a reasonable approach. However a number can have more than one kind of ending.

The fact that we usually write in base 10 does not prevent a base 10 number from having a base n ending. For example, if we divide the base 10 number 249 by 10, the remainder is 9 (the base 10 ending). However this fact does not prevent us from considering the base 7 ending (remainder), which is 4.

In this section, we will explore a more efficient data compression technique, **DCB**, or **Decimal Coded Binaries** (which are not the same as the binary coded decimals of computer science). As the name suggests, DCB hybridizes the base 10 and base 2 number systems. We will see that DCB quantities can be thought of as base 10 numbers with base 2 endings.

In the <u>ordinary</u> significant figure theory of the binary number system, the minimum estimated measurement uncertainty (Um) allowed on the last reported digit is  $\pm 0.5$ , as in base 10, but the maximum Um on the last reported digit is  $\pm 1$ . However we will use a  $\pm 2$  to  $\pm 4$ rounding convention in order to guarantee that the rounding ratio is always at least 4, thereby minimizing the rounding error. (The minimum rounding ratio for all of our data compression techniques is 4.) Therefore after we round off a binary number (using the  $\pm 2$  to  $\pm 4$ convention), it will have uncertainty on the last three significant binary digits.

In some ways, binary significant figures are nicer than base 10 significant figures. In binary, the estimated measurement uncertainty on the last reported digit is limited to a  $\pm 4/\pm 2 = 2$ -fold range, as compared with a ten-fold range for base 10. The major disadvantage of binary numbers is that they require too much space to write out. For example, "512" in base 10 is "1 000 000 000" in binary. However it is possible to combine the virtues of the base 10 and binary number systems, and have the best of both worlds.

Basically, the DCB algorithm converts an **integerized**\* base 10 quantity into binary, rounds to the correct number of binary digits, and then converts back to base 10. We can represent this concept as "2-R-10" in symbolic shorthand. However there is one difficulty with this oversimplified picture, which we will illustrate in the next paragraph.

Suppose that the value of a measurement is 302 mg, and that only two significant figures can be justified, which means that we must round to 300 mg. How is a third party to know which, if any of the

\*For now, our explanation of **integerization** will be slightly oversimplified. The number 0.0345 is  $3.45\times10^{-2}$  in scientific notation. Remember that we are calling the "3.45" the **mantissa**. The **integerized** mantissa is 345, and the **integerized** form of the original number is  $345\times10^{-4}$ . terminal zeros in "300" are significant figures? This is the **terminal zero problem**.

There are two ordinary ways to deal with this situation. First we could express the quantity as " $3.0 \times 10^2$  mg", using scientific notation. Alternatively we could write "0.30 g". Neither approach will solve the terminal zero problem for DCB. Instead we will use a binary **marker** as an uncertainty location bit. The full-fledged algorithm for converting base 10 data to DCB notation is as follows:

- 1) <u>Integerization</u>. Let **M** and **Um** represent the absolute value of the mean of a series of measurements, and its standard error, respectively.
  - (a) If Um of M is less than 4, then multiply both M and Um by 10. Repeat as needed, until the Um becomes ≥ 4.
  - (b) Set a counter variable J (which is initially zero) equal to the number of times (a) is repeated.
  - (c) and (d) These steps (to be given later) are used only with a DCB variation called **Scientific DCB**.
- 2) <u>Convert</u> the integerized (base 10) M to binary.
- 3) <u>Round</u> the result of Step 2 such that the adjusted Um on the last significant binary digit is between 2 and 4. Be sure to remember the position of the last significant binary digit!

The fifth step will be to convert back to base 10, but there is one hurdle to clear first. Suppose that the result of Step 2 is 11011000 in binary (216 in base 10). How is a third party to know which binary digit is the last significant figure? It could be the right-most "1" or it could be any of the three final zeros. We have come back to the **terminal zero problem**, which we will solve by flagging the location of the final significant binary digit.

4) <u>Flagging</u>. Put a "1" immediately after the last significant binary digit, and keep it there.

This means that the right-most "1" has absolutely nothing to do with the actual value of the number, and is merely a **marker**, which says that there is uncertainty on the next three binary digits to the left.

- 5) <u>Convert</u> the result of Step 4 <u>to base 10</u>. (This will always be an integer.) The marker is now a part of the new base 10 number.
- 6) <u>Bookkeeping.</u> Take the result of Step 5 and move the decimal point J places to the left (or -J places to the right). Do not discard or add any terminal zeros when moving the decimal point. If necessary, express in a scientific-like notation. If the measurement's sign is negative, then remember to put a (-) sign in front of the DCB quantity.

This completes the procedure for translating the results from a set of scientific measurements (i.e. the mean value and its uncertainty) into DCB notation. We may summarize the complete DCB coding procedure as

"Int-2-R-F-10-B". A listing of the programs for coding and decoding DCB on the HP15C calculator may be obtained by writing to the authors.

There is one important boundary condition for DCB. This notation can only be used to represent a quantity, whose standard error of the mean is less than the absolute value of the mean. Now we will give some examples.

Our first example will serve two purposes. First we will get some practice in decoding DCB (i.e. translating DCB into prose). Secondly we will gain some insight into the importance of terminal zeros.

## Example 1.

Let A = 2.3 and B = 2.30, both in DCB notation. Is A equivalent to B? Working backwards, we will translate A into prose.

Obviously J =1, and the Step 5 result is 23 (in base 10).

The Step 4 result is 10111 (in binary).

The marker in "101111" is in the ones' place. This means two things.

- (a) There is uncertainty in the twos', fours', and eights' places; i.e. that the adjusted Um is between  $\pm 4$  and  $\pm 8$ .
- (b) The Step 3 result (rounded binary quantity without marker) is 10110.

We do not know the value of the Step 2 result (except that it is between binary 10101.1 and binary 10110.1), because a little information was lost in rounding. So we will use the rounded value, 10110.

The Step 1 result is 22 in base 10.

Since J = 1, we divide both "22" and the adjusted Um by  $10^1$  in order to arrive at the prose equivalent of A, which is "2.2, with an estimated measurement uncertainty between 0.4 and 0.8". (Note that "between 0.4 and 0.8" is not a confidence interval.)

Similarly, it can be shown that B has a prose equivalent of "2.28, with an estimated measurement uncertainty between 0.08 and 0.16". Therefore A is not equivalent to B. This is why we must be so careful with terminal zeros when we are using DCB.

If one is doing arithmetic on DCB numbers, then each quantity should be decomposed into its actual value and uncertainty. Thus there are four distinct operations to perform:

- 1) the decomposition (decoding)
- 2) the calculation itself
- 3) a propagation-of-uncertainty analysis
- 4) combining (coding) the results of (2) and (3) into a single DCB quantity.

Since a DCB quantity looks like an ordinary base 10 number, it is possible to confuse the two. If one is constructing a table of scientific data, using DCB notation, then it would be best to state this explicitly at the outset.

If the person reading such a table is not familiar with DCB, and mistakes a DCB quantity for an ordinary number, then he or she loses out on the information about the uncertainty. However the value of the measurement does not suffer much, as we will see in the next example.

# Example 2.

Suppose that the mean value of a series of measurements is 35.20 mV, and that the systematic error is assumed to be negligible in comparison with the standard error of the mean, which is 0.71 mV.

- 1a) Um = 0.71 < 4. Therefore the adjusted mean is 352, and the adjusted Um is 7.1.
- 1b) J = 1
- 2) The (base 10) number 352, expressed in binary is 101100000.
- 3) This is rounded to the correct number of binary digits already.
- 4) The last significant binary digit is the second "0" from the right, in the twos' place. Therefore we will replace the right-most "0" with a "1" (the marker). The result is 101100001.
- 5) Converting the result of (4) back to base 10 gives 353.
- Moving the decimal point J (=1) places to the left yields 35.3 mV, in DCB notation.

Comparing this result with the original base 10 quantity, we see that the two numbers (35.2 and 35.3) are quite close. In general, their difference will be no greater than Um/4; i.e. the penalty is small when one mistakes DCB for prosaic notation. Thus DCB is very forgiving (but not as forgiving as Linear Code).

For many data tables—such as reduction potentials—where most of the values are in the same ballpark, DCB notation will be adequate. However it would be rather cumbersome to use DCB <u>per se</u> in tables of equilibrium constants. For data tables, which would ordinarily require scientific notation, there is an alternative, **Scientific DCB (SDCB)**. This is very similar to DCB, but is a scientific-like notation. In Scientific DCB, the following additions are made to the DCB procedure.

## Scientific DCB Addenda:

- 1c) If Um  $\geq$  40 then divide the base 10 quantity (and Um) by 10. Repeat as needed.
- 1d) Let J = -1 multiplied by the number of times 1c is repeated (if 1a does not apply).

In the next several paragraphs, we will discuss the comparative economics of Scientific DCB. We are considering Scientific DCB rather than DCB, because DCB, like **un**scientific notation, can be rather wasteful. (Imagine having to write the Avogadro constant that way!) Going back to Example 2, the original base 10 quantity in ordinary scientific notation, used in conjunction with ordinary stand-alone significant figures, would be expressed as  $3.5\times10^{1}$  mV, which requires one less digit than Scientific DCB notation ( $3.53\times10^{1}$  mV).

Scientific DCB and scientific notation (used in conjunction with ordinary stand-alone significant figures) will have the same digital cost only when Um on the last significant base 10 digit is between 4 and 5. The probability of this being the case is

# $\log(5/4) = 0.09691$

Therefore the absolute cost of Scientific DCB is

# 1 - 0.09691 = 0.90309 digits

Obviously Scientific DCB is cheaper than Linear Code, whose cost is 1.60206 digits, but linear code gives more information about Um. In linear code, Um can be pinned down within a  $10^{0.1} = 1.26$ -fold range, as compared with a two-fold range <u>at worst</u> for Scientific DCB. (If the binary marker of an SDCB quantity is in the fours' place, then the estimated uncertainty is pinned down within a 40/32 = 1.25-fold range.)

However we can construct **Extended DCB** (a modification of Scientific DCB), which will allow us to make a fair comparison between the two methods of data compression. In order to demonstrate that SDCB is a more efficient technique than Linear Code, we will show that <u>Extended</u> DCB gives more information about the estimated uncertainty, and is cheaper than Linear Code. Since complete mastery of Extended DCB is not necessary for the reader who wants a general understanding of DCB, we will give only a brief outline of Extended DCB.

Modifications to SDCB Procedure for Extended DCB .

- A. Change the magic numbers in Step 1 of the SDCB procedure from 4 and 40 to 16 and 160.
- B. Reserve the last two binary digits in the Step 4 result for a quaternary uncertainty code, analogous to the base 10 uncertainty code used for linear code in the previous section. The result is an SDCB-Linear Code hybrid, Extended DCB.

Extended DCB will allow us to pin down Um within a  $2^{1/4} = 1.19$ -fold range <u>at worst</u>, an improvement over linear code. The additional cost of Extended DCB (over Scientific DCB) is

## $\log 4 = 0.60206 \text{ digits}$

Thus the total cost of Extended DCB is

## 0.90309 + 0.60206 = 1.50515 digits

which is cheaper than Linear Code. We have seen that when Scientific DCB is linearized, the resulting code is more economical than Linear Code alone. It would be reasonable to infer that it was the Scientific DCB component which contributed the increase in cost-effectiveness. Therefore Scientific DCB is inherently more economical than Linear Code.

Thus DCB is an efficient and forgiving technique. The essence of DCB is to combine the compactness of base 10 with the uncertainty specificity of binary. A mnemonic for the DCB algorithm is "Int-2-R-F-10-B".

In a later section, we will see that the DCB variations have an additional virtue, flexibility. We will argue that DCB is a better overall technique than Linear Code.

#### EXPERIMENTAL SECTION

In an attempt to integrate the theory of decimal coded binaries with the real world, the DCB algorithm was programmmed into an AIM 65 microcomputer, which was interfaced with an Orion 701A lonalyzer (pH meter), via its digital output edge connector. The program, which was written in (interpreted) BASIC, included a machine language subroutine for reproducibly recognizing when practical equilibrium would have been attained, had the apparatus been used with an actual sample solution.

Measurements of pH were simulated by means of the calibration knob on the Orion. The uncertainty for a given simulated measurement was manually entered from the keyboard of the AIM. It would have been just as easy (albeit much more time-consuming, because of the practical equilibrium subroutine) to arrange for the program to calculate the standard error of the mean from a series of measurements. After taking the data, the program expressed the result in a DCB format.

Table VI shows the details of the hardware interfacing.

Table VI	Connections Between the AIM 65 Microcomputer and the Orion 701A lonalyzer		
AIM 65	ORION 701A		
PB0	.1		
PB1	.2		
PB2	.4		
PB3	.8		
PB4	1		
PB5	2		
PB6	4		
PB7	8		
PA0	10		
PA1	20		
PA2	40		
PA3	80		
PA4	100		
PA5	200		
PA6	400		
PA7	800		
CA1	DATA READY		
CA2	HOLD		
GROUND	GROUND		

#### **RESULTS AND DISCUSSION**

~

The entire program was well within the AlM's 4K of memory. About a minute was required for the recognition of practical equilibrium. After that, the program took only a few seconds to combine the simulated mean and simulated standard error of the mean into a DCB number (in an integerized scientific-like notation), which could be viewed in the AlM's LED display. This experiment demonstrates that the computer interfacing requirements of DCB do not pose a major problem in the implementation of this data compaction technique. Even if the innards of a given chemical instrument are not readily accessible, DCB coding and translating routines can readily be programmed into an HP15C calculator.

# SUMMARY AND CONCLUSION

We have introduced two classes of data compression techniques: Linear Code and Decimal Code Binaries (DCB, Scientific DCB, and Extended DCB). Either method can provide a readable and economical format for reporting the two essential components of a scientific measurement—the measurement itself and an index of its trustworthiness.

Now we will compare the relative merits of linear code and DCB. These two methods will be evaluated in terms of the following criteria:

- 1) Efficiency
- 2) Flexibility
- 3) Forgiveness
- 4) Simplicity

Using a linguistic parable, we compared linear code with the data compaction techniques used in an ordinary telegram, while DCB was compared with the use of vocal inflection, the latter approach being somewhat more efficient. The next example will illustrate the **flexibility** of DCB.

<u>Example 3</u>. Experimental mean = 123456 bacteria/L. The standard error of the mean (Um) is 789 bacteria/L.

Linear code	1.2355X10 <sup>5</sup>	bacteria/L
DCB	123520	bacteria/L
Scientific DCB	1.235X10 <sup>5</sup>	bacteria/L

Example 3 shows that it is sometimes necessary to use a scientificlike notation with linear code. This is because of the terminal zero problem, which we discussed in an earlier section. In principle, it will always be possible to express DCB quantities in ordinary unscientific notation, which is highly readable in data tables. However we have the option of using Scientific DCB if we want to save space when constructing tables of widely spaced quantities, like solubility products.

Both linear code and DCB are forgiving, in the sense that the reader of scientific data tables does not suffer much if he or she has never even heard of these coding techniques, since the value of the measurement-based quantity is distorted very little in the coding process. Of course the information about the measurement's uncertainty is available only to those who know that it is there! We have already pointed out that DCB is more forgiving than linear code.

Conceptual simplicity is the least important of the four criteria. Since coding and decoding procedures for DCB can be programmed into an HP15C calculator, the user of the technique need not worry about the fine details. Since linear code is merely doing the obvious, it is more understandable than DCB, although DCB programs tend to be short (about 100 bytes for both coding and decoding in an HP15C calculator). Table VII graphically summarizes this comparison.

Table VII	A Comparison of DCB with Linear Code.			
	Efficient	Flexible	Forgiving	Simple
Linear code DCB variations	¥ ***	* ***	** *	×× ×

Table VII shows that DCB is a better method in most respects. Linear Code serves as a learning tool, as an auxilliary technique, and as a Brand X or reference method, which highlights the attractive features of the more sophisticated technique, DCB. In the next several paragraphs, we will discuss the potential role of DCB in science and technology.

At present, there is a double standard among scientists about the reporting of measurement data. On the one hand, we pay lip service to the idea that we should always include an estimate of the uncertainty, when we report a measurement. Yet we tend to forget this when we publish our data in tabular form—and for good reason. A data table would be rather cluttered if we included a detailed error analysis for each datum.

In some circumstances, the present practice is tolerable. If a chromatographer is reading a table of GC retention indices, then he or she will probably have some feeling for the limitations of the measurements, even if the uncertainties are not stated explicitly.

However an organic chemist may be using these tables to assist in the identification of a newly synthesized compound. He or she will want to compare his or her retention index (for a given stationary phase) with the literature value. The question is: "How close is close enough?" This will not be a problem if the literature value is reported in a DCB format.

When we put our data into tables, DCB will allow us to practice what we preach about the reporting of uncertainty. DCB is the middle ground between stand-alone significant figures and the prosaic reporting of measurement data. It is very efficient at communicating the essentials of measurement data. Thus far, we have emphasized the saving of ink. However the potential uses of DCB extend far beyond the printed page.

In the previous section, we argued that the programming and computer interfacing requirements of DCB are not prohibitive. DCB could improve the efficiency of scientific data storage in computer memory (or on a hard disk or on a floppy). Moreover there is no reason to preclude the use of standard data compression techniques in tandem with DCB. If DCB promotes more efficient use of computer memory, then it should also increase the speed of electronic communication. Let's take an example.

Suppose that NASA sends a probe to Titan (a satellite of Saturn), and that there are 100 experiments running simultaneously inside the landing module. It would be important to transmit the data to Earth as rapidly as possible. DCB (or even Hexadecimal Coded Binaries) could be an important part of the overall plan to optimize the communication rate, by combining in one signal both the datum and the value of the measured noise.

Of course the potential applications of DCB are not limited to the exploration of outer space. The usefulness of most chemical instruments with digital readout could be enhanced if DCB was a built-in feature.

In large projects, technicians are often sent out into the field with portable chemical instruments. The logging time could be reduced if the technician wrote a single DCB number into his or her notebook, rather than having to write both a mean and its standard error.

In this paper we have presented two new techniques for compressing scientific data—DCB and linear code. The best method, DCB, does not have a very high level of specificity for the uncertainty. If more information about uncertainty is required for a given application, then a tailor-made technique could easily be constructed, by hybridizing DCB and linear code, as we did with Extended DCB in an earlier section. Therefore DCB is really an <u>array</u> of techniques.

To summarize, DCB should increase the effectiveness of automated communication---written and electronic---among scientists, especially across disciplinary boundaries.

#### APPENDIX

Both classes of data compaction techniques discussed in this paper combine a measured quantity and its uncertainty within a single number. In contrast with ordinary stand-alone significant figures, these techniques have a high level of specificity for the uncertainty. It would be of interest to be able to do a simple propagation-ofuncertainty analysis on a calculation involving quantities which have been coded by either method.

For example, in the second section we introduce the Linear Coding technique. If two Linear-Coded quantities are multiplied together, it would be nice to be able to express the product in Linear Code also. This will be possible only if we have chosen a definition of uncertainty, which permits straightforward propagation-of-uncertainty analysis.

We will argue that propagation of uncertainty is quite simple for the absolute limit of error and standard error of the mean definitions of uncertainty, but that there are serious problems with the confidence interval definition, because the sample size must be taken into account.

If uncertainty is defined to be the absolute limit of error, then propagation of uncertainty can be handled by the following equation:

### $RU = \Delta f / f = [\Sigma(df/dx_i)\Delta x_i] / f + RUM$ (A.1)

where **RU** is the relative uncertainty of **f** (a function of the  $x_i$ ),  $\Delta f$  is the absolute value of the uncertainty of f,  $\Delta x_i$  is the absolute value of the uncertainty of  $x_i$ , and **RUM** is the relative uncertainty of the calculation method. Sometimes the functional relationship f is only approximate and is itself a source of error. (For example Beer's Law neglects the effect of stray light.) It is also assumed that f is well behaved, and that each  $\Delta x_i$  is small relative to  $x_i$ .

If uncertainty is defined to be some multiple of the sample standard error of the mean, then we may use the following equation:

$$U = A\Delta f = A\{\Sigma[(df/dx_i)\Delta x_i]^2\}^{1/2}$$
(A.2)

where **U** is the uncertainty,  $\Delta f$  is the absolute value of the estimated standard deviation of f, each  $\mathbf{x_i}$  is the mean value of a series of measurements (of the same parameter),  $\Delta \mathbf{x_i}$  is the absolute value of the standard error of the mean of  $\mathbf{x_i}$ , and **A** is a positive real number. Thus propagation of uncertainty is very simple for both the absolute limit of error and standard error of the mean definitions of uncertainty, because Equations A.1 and A.2 are independent of sample sizes and of the component frequency functions (i.e. it doesn't matter whether they are Gaussian, Poisson, rectangular, etc.).

If uncertainty is defined to be half the span of a 95% confidence interval, then the propagation of uncertainty is dependent on the sample size and frequency function associated with each of the  $x_i$ . The implication is that in this case, there is no simple formula for propagation of uncertainty, which will work for all cases. To prove this rigorously would be beyond the scope of our present discussion. However in the next several paragraphs we will explore the obvious approaches. All of these blind alleys will become "the exceptions which prove the rule". Let's suppose that

- (a) the data points for each of the x<sub>i</sub> are normally distributed, and
- (b) the sample size is known for each of the  $x_i$ .

Then we may use a t Table to help us calculate each of the standard errors of the mean  $(\Delta x_i)$ , which we plug into Equation A.2 in order to find  $\Delta f$ . But then how do we calculate the 95% confidence interval for f? There are two obvious possibilities.

If the  $\Delta x_i(df/dx_i)$  are all equal, and if the sample sizes (of the calculation's components) are all equal, then the calculation of the confidence interval will be a radial error problem, which can be solved using a chi-square technique<sup>13</sup>.

On the other hand, the t Table can be used in this final step only if we can make the simplifying assumption that essentially all of the uncertainty is contributed by a single **least precise factor**, **x**. However in this special case, there is no need for a t Table, or for assumptions (a) or (b). Instead we may use the following equation:

$$\Delta f = \Delta x (df/dx) \qquad (A.3)$$

with  $\Delta x$  and  $\Delta f$  representing the half-spans of the 95% confidence intervals of x and f, respectively.

An even bigger problem is that the sample sizes will not always be available when we are using other people's data in our calculation.

There is a simple way to obtain a confidence interval for the result of a calculation, but it will not be the 95% confidence interval. In the following artificial example we will suppose that the measured base and height of a rectangle are 987 cm and 654 cm, respectively, that the 95% confidence interval of each quantity is  $\pm 1$  cm, and that no information is available about sample size. The estimated area is

# $987 * 654 = 645498 \text{ cm}^2$

From the definition of the 95% confidence interval, the compound probability that the base is greater than (987+1) cm, and that the height is greater than (654+1) cm is

### $[(1 - 0.95)/2]^2 = 6.25 \times 10^{-4}$

which is also equal to the probability that the 95% confidence intervals fail to bracket <u>both</u> base and height at the low ends. Therefore the probability P that the true mean area (i.e. the calculated area, based upon the true mean values of the base and height measurements) is <u>not</u> bracketed by the interval

# [(654 - 1)(987 - 1), (654 + 1)(987 + 1)] = [643858, 647140]

may be calculated as follows:

$$P = 2(6.25 \times 10^{-4}) = 1.25 \times 10^{-3}$$

Thus the above interval is the

confidence interval for the true mean area of the rectangle. However we were seeking the <u>95%</u> confidence interval.

Again, we have failed to find a general method for obtaining the 95% confidence interval for f, from the 95% confidence intervals of the  $x_i$ . If such a method does exist, then it is not obvious. It would be of theoretical interest to find such a method, or to prove its nonexistence. However the main point of this discussion is that propagation of uncertainty in the general case is very simple for the standard error of the mean and the absolute limit of error definitions of uncertainty, but it is not straightforward for the confidence interval definition.

# DCB PROGRAMS FOR THE HP15C SCIENTIFIC CALCULATOR

Since HP15C programming is rather primitive, there are some limitations, which we must contend with. There are no character variables, nor is there any string manipulation. In particular, the calculator cannot recognize a terminal zero in a decimal fraction; i.e. it cannot distinguish between "1.2" and "1.20". Therefore at times the directions will tell you to ignore decimal points, to pretend that real numbers are integers. At other times, the instructions will tell you how to use your common sense in order to put the decimal point in its proper place. Since the simplest concepts are often the most difficult to explain, the directions may seem more complicated than they really are.

### Program for Expressing Measurement Data in a DCB Format

This first program transforms experimental data into DCB notation. We will give instructions for using the program before listing the program itself. Suppose that you are taking a series of measurements of the same thing (eg. the spectrophotometric absorbance of a solution).

- A. First key in "f  $\Sigma$ " to clear the statistical registers of the calculator.
- B. Enter the measurements or their <u>mantissas</u><sup>\*</sup> into the calculator, as you would enter ordinary statistical data using the  $\Sigma$ <sup>+</sup> key after each entry.

Most of the time you will have the option of entering the measurements themselves, rather than their mantissas. However if the numbers are very large (in the neighborhood of 10<sup>9</sup>), then you may get a spurious result. If you use mantissas (the safest approach), then you will also get the maximum compression of your data.

\*For example, the mantissa of the Avogadro constant is "6.022".

<u>Common sense</u>. If you are using the measurement mantissas rather than the measurements themselves, then all of the measurements, when expressed in scientific notation, should have the same exponent. If they do not, then it will be necessary for you to force them all into the same mold.

The program, which has a bad case of integer obsession, will sometimes ignore the decimal points in nonintegers. Therefore you may need to do some scaling up or scaling down after the program has finished running.

- C. When all of the measurement data has been entered, then key in "f C". "C" (which stands for "Coding") is the name of the program.
- D. After about 7 seconds, the <u>integerized</u> DCB mantissa (the DCB mantissa without the decimal, which is understood to be between the first and second digits) will be displayed.
- E. The final DCB quantity is the displayed mantissa, with a decimal point inserted between the first and second digits, followed by the exponential part (the X10?).

Do <u>not</u> add or discard any terminal zeros! For example, if the number in the display is "180", then the DCB mantissa may be written as "1.80". Do <u>not</u> write "1.8". The DCB quantities "1.80" and "1.8" have completely different meanings.

- F. Write the complete DCB quantity into your lab notebook. If this can be done without adding any terminal zeros, then you have the option of using an ordinary **un**scientific DCB notation. However a scientific-like notation, which includes both a DCB mantissa and an exponential part, is always correct.
- G. If you are constructing a data table using DCB notation, then you should state this explicitly in the heading of the table. Then your readers will not confuse it with ordinary notation, and they will be able to take full advantage of the information about the measurement's uncertainty embedded within the DCB quantity.

The algorithm has two boundary conditions. If the absolute value of mean is much smaller than its standard error, then it will not be possible to express the result in DCB notation. In particular, the

program will not handle a zero mean. Secondly, it is not possible to express an exact number (having zero uncertainty) in DCB notation.

<u>Example</u>. Suppose that the values of three voltage measurements were 0.496 mV, 0.508 mV, and 0.520 mV. These numbers can be entered into the calculator

- (a) without modification
- (b) or as 4.96, 5.08, and 5.20 respectively, with X10<sup>-1</sup> understood
- (c) or as 49.6, 50.8, and 50.2 respectively, with  $\times 10^{-2}$  understood
- (d) or as 496, 508, and 520 respectively, with  $\times 10^{-3}$  understood.

In each case, the integerized DCB mantissa displayed by the calculator will be "510" (which is understood to mean  $5.10 \times 10^{-1}$ ). The DCB quantity, which you put into your lab notebook can be written in any of the following ways:

- (a) 0.510 m∨
- (b) 5.10X10<sup>-1</sup> mV
- (c) 51.0X10<sup>-2</sup> mV
- (d)  $510 \times 10^{-3} \text{ mV}$

There is one main pitfall: Do not discard the terminal zero! The following is the annotated program:

	X register	Y register	Z register
Preliminaries	-	-	-
1 fLBL C			
2 fFIX 0			
3 g <del>x</del>	x		
Handles the boundary co	ndition where $\overline{\mathbf{x}}$	might be < 0.	
4 ENTER	x	x	
5 g ABS	X	x	
6 STO 1			
7 ÷	Sign (x)		
8 STO 8	-		
Formatting $\overline{\mathbf{x}}$ and standa	rd error of the i	mean.	
9 g s	S		
10 RCL 2	Ν	S	

12	√× ÷	√N Std. error	S
	STO 0		
14		4	Std. error
	x≓y	Std. error	4
	g TEST 9 (x ≥ y)		
	GTO 0		
18		4/std. error	
	g LOG	log	
20		1	log
21		1 + log	
	g INT	exponent	
	10×	factor	
	STO X 1		
	RCL X 0	std. error	
	ding Range Index		
	f LBL 0		
	g LOG	log std. error	
28		2	log std. error
	g LOG	log 2	log std. error
30		base 2 log of s	ta. error
	g INT	Range Index	
32	inding	1	RI
33		Adjusted RI	ni
34		2	ARI
	z x ≓ y	ARI	2
36	-	AR	۷
	STO I	An	
	RCL 1	x	AR
	x≓y	AR	X
40	-	Shrunk X	
41			
42	5	.5	Shrunk x
43		Intermed	
	g INT	RS x	
	RCL I	AR	
46		Rounded X	

Binary Marker			
47 RCL I	AR	Rounded <del>x</del>	
48 2	2	AR	Rounded X
49 ÷	Marker	Rounded X	
50 +	DCB		
51 RCL 8	Śign (x)	DCB	
52 X	Voila!		
53 g RTN			

# HP15C Program for Decoding DCB.

This second program translates DCB into plain English. Again, we will give instructions on the use of the program before we actually list it.

- A. Key in the <u>integerized</u> DCB mantissa (i.e. the mantissa with the decimal point omitted, but understood to be between the first and second digits).
- B. Key in "f D". The "D" is a mnemonic for "Decode", and is the name of the program.
- C. The integerized mantissa of the mean will appear in the display (X register). The Y register will contain the estimated relative uncertainty (estimated standard error of the mean divided by the sample mean).

The resolution of DCB is such that the <u>estimated</u> relative uncertainty in the Y register will not differ from the <u>calculated</u> value of the relative uncertainty by more than a factor of  $\sqrt{2}$  $\approx 1.414$  (not to be confused with a confidence interval). If you want to view more than one significant figure of the estimated relative uncertainty, then you will need to key in "f PREFIX" (or fiddle with "f FIX" or "f SCI").

The following is the actual program listing:

1 f LBL D2 q x = 0

Avoiding an

3 GTO 2 infinite loop. 4 f CLEAR REG Initialization. **5** ENTER Handles any 6 g ABS DCB quantity 7 ÷ even if 8 STO 8 it is less 9 gLST X than zero. 10 STO 0 11 f LBL 1 12 2 Is the 13 ÷ number 14 f FRAC divisible 15 g TEST 0 by 2? 16 GTO 2 If no, branch down. 17 1 Otherwise 18 STO + I increment counter 19 gLSTX and 20 GTO 1 loop back. 21 f LBL 2 22 2 No. of clean 23 RCL I divisions by 2 as 24 Y<sup>X</sup> exponent of 2. 25 STO 1 26 CHS Subtract out the 27 RCL + 0 binary marker. 28 RCL 1 Estimation 29 3 of the 30 2 standard 31 1/x error 32 √x of the 33 ÷ mean. |mean| in X register; estimated standard error in Y reg. 34 x ≓ y Estimated relative uncertainty (ERU) **3**5 ÷ 36 g LST X |mean| in X register; ERU in Y register 37 RCL 8 38 X Mean in X register; estimated standard error in Y reg. 39 f FIX 0 40 g RTN

#### THEORY

Eight Code is the most complicated and most efficient of the data compaction methods in this study, although it is less forgiving and less flexible than DCB. Before giving the Eight Code algorithm, we will discuss the general principles of this technique. Even these may seem bewildering at first. However the BASIC coding program occupies about 1K of memory in an eight bit microcomputer (and about 120 bytes in an HP15C scientific calculator). Therefore it is possible to make practical use of the technique, if one has a good understanding of its purpose.

Eight Code relies heavily on the **modulo** concept. "Q modulo N" means: "Divide the quantity Q by N, and take the remainder." As the name suggests, Eight Code uses "modulo 8".

In Eight Code, **mantissa** is also an important concept. The mantissa of the Avogadro constant  $(6.022 \times 10^{23} \text{ mol}^{-1})$  is "6.022". At times, we will find it convenient to think of mantissas as being integers. For example, the integerized mantissa of the Avogadro constant is "6022".

As with Linear Code, and especially with DCB, the numerical value of the coded quantity will be fairly close to that of the actual experimental result. However no information about the estimated measurement uncertainty Um is available unless one knows the coding method (or has programmed it into his or her scientific calculator). In order to obtain information about Um from Eight Code, one must look at the coded integerized mantissa, modulo 8, which we will call the **mod value**.

In Linear Code, the final base 10 digit is the uncertainty code. Similarly in DCB, the final binary "1" serves as the marker, or uncertainty location bit. Both the uncertainty code (in Linear Code) and the marker (in DCB) give information only about the estimated measurement uncertainty (Um). The efficiency and complexity of Eight Code stem from the fact that the mod value has a two-fold purpose; it gives information about Um and about the measured quantity. There are eight integral mod values, corresponding to four categories of uncertainty (on the last digit of the coded integerized mantissa). **Class 1**, the category of highest uncertainty, corresponds to a mod value of zero. **Class 2**, the second-highest uncertainty category, corresponds to a mod value of 1. Mod values of two and three correspond to **Class 3**, the third-highest uncertainty category. **Class 4**, the category of lowest uncertainty, corresponds to mod values 4 through 7.

Notice that it is possible to represent Class 4 (or Class 3) by more than one mod value. The apparent redundancy of Eight Code allows the measured quantity itself to have two extra binary digits for Class 4 uncertainties, and one extra for Class 3 uncertainties. The rationale for doing this is the following general principle:

The smaller the relative uncertainty, the larger the number of significant figures.

The Eight Code procedure is as follows:

- Preliminary integerization. (This is exactly the same as Step 1 in the Scientific DCB procedure given in a previous section.) Let M and Um represent the absolute value of the mean of a series of measurements (of the same parameter), and its estimated measurement uncertainty (standard error of the mean), respectively.
  - (a) If Um of M is less than 4, then multiply both M and Um by 10. Repeat as needed, until the Um becomes ≥ 4.
  - (b) Set a counter variable J (which is initially zero) equal to the number of times (a) is repeated.
  - (c) If  $Um \ge 40$  then divide the base 10 quantity (and Um) by 10. Repeat as needed, until the Um becomes < 40.
  - (d) Let J = -1 multiplied by the number of times (c) is repeated if
     (a) does not apply.
- 2) Let **AM** = 10<sup>J</sup> times M. <u>Round</u> AM to the nearest multiple of 8. We will call this result **ARM** (the Adjusted and Rounded Mantissa).
- 3) If adjusted Um  $\geq$  8, then go to Step 4.

Steps 3 to 5 do the actual coding.

- (a) If  $2 \leq AM ARM$  then add 7 to ARM.
- (b) If  $0 \le AM ARM \le 2$  then add 6 to ARM.
- (c) If  $-2 \leq AM ARM < 0$  then add 5 to ARM.
- (d) If AM-ARM < -2 then add 4 to ARM.

- 4) If adjusted Um  $\geq$  16, then go to Step 5.
  - (a) If  $0 \le AM ARM$  then add 3 to ARM.
  - (b) If AM ARM <0 then add 2 to ARM.
- 5) If  $16 \leq Um \leq 25.3$  then add 1 to ARM.
- 6) <u>Bookkeeping</u>. Take ARM and move the decimal point J places to the left (or -J places to the right). Do not discard or add any terminal zeros when moving the decimal point. If necessary, express in a scientific-like notation. (This step is esentially the same as in the DCB variations.)

In the next example, we will work through the Eight Code algorithm, starting with the mean and standard error of the mean for a series of hypothetical chemical measurements. We will also see that Eight Code is not as forgiving as DCB.

Example. Mean = M = 11.3; Um = 0.5

- 1) AM = 113; adjusted Um = 5; J = 1
- 2) ARM = 112
- 3) Adjusted Um < 8. Steps 4 and 5 do not apply.
  - (a) does not apply
  - (b)  $0 \le AM ARM = 113 112 = 1 \le 2$  Therefore we add 6 to ARM and obtain 118. Substeps (c) and (d) do not apply.
- 6) Therefore the experimental result, expressed in Eight Code is 11.8.

If we had used DCB in the above example, instead of Eight Code, then the coded result would have been "11.4". The ordinary number "11.4" is closer to the original measurement. In general, the penalty for <u>not</u> knowing the code is smaller for DCB, and smallest for Linear Code.

Example. M = 239 mV; Um = 3 mV

The experimental result expressed in Eight Code is 239.2 mV.

Now we will work backwards; i.e. we will translate from Eight Code into prose.

The coded integerized mantissa is 2392, and J = 1.

The ordinary number 2392 modulo 8 is zero.

Since the mod value is zero, Steps 3 to 5, which assign mod values 1-7, and which cover the uncertainty range  $\pm 4$  through  $\pm 25.3$ , do not apply.

This means that the uncertainty on the final "2" (in 239.2) is between  $\pm 25.3$  and 40, by default.

Therefore the prose value is "239.2, with an estimated measurement uncertainty between  $\pm 2.53$  and  $\pm 4$ ". (Remember that this is <u>not</u> a confidence interval.)

As an exercise, it might be helpful to work backwards through the first example.

We will see that Eight Code is slightly more cost-effective than Scientific DCB. In comparing the economics of the two techniques, we will emphasize two elements—digital cost and uncertainty resolution.

Step 1 is identical for both techniques. This integerization step determines digital cost. Therefore the digital costs of Eight Code and Scientific DCB are the same.

The uncertainty resolution of Eight Code is slightly better than that of Scientific DCB. In Scientific DCB, the estimated measurement uncertainty (Um) can be located within a two-fold range, except when the binary marker is in the eights' place, in which case Um is pinned down within a 40/32 = 1.25-fold range.

We could have defined Eight Code such that the specificity for the uncertainty would be identical to that of Scientific DCB, by changing the second magic number in Step 5 of the Eight Code procedure from 25.3 to 32. However it is more efficient to have the <u>non-two-fold</u> range divvied up evenly between two uncertainty categories. (This results in two 1.58-fold ranges, and two two-fold ranges.) Thus Eight Code has a slight edge over Scientific DCB, in terms of efficiency.

All things considered, DCB is a better technique than Eight Code. Eight Code is slightly more efficient, but DCB is more forgiving, more flexible, and simpler than Eight Code. In hindsight, the real significance of Eight Code is as a prototype for future techniques, which are beyond the scope of the present research.

### EXPERIMENTAL AND RESULTS SECTION

The efficacy of Eight Code was tested in an experiment, in which an AIM 65 microcomputer was interfaced through an in-house, analog-todigital converter\* to the output of a Perkin-Elmer LC-55 single beam spectrophotometer. As in the DCB experiment, measurements were simulated by twiddling the adjustment knobs.

The BASIC interfacing and coding program was well within the AIM's 4K of memory. The interfacing part of the program was a built upon the skeleton of a program called "DVM", courtesy of Michael Schuyler. (See the Appendix chapter.)

The BCD (not DCB!) signal from the A-to-D converter was outputted to the microcomputer. The BASIC program took a series of measurements, and combined the mean and its standard error into a single Eight Code quantity. The computation time was only a few seconds in each case. On the whole, Eight Code and DCB were equally easy to implement. The experimental results were printed out on computer tapes, and copies of these tapes are listed in the Appendix chapter. The Appendix chapter also contains Eight Code programs for the HP15C scientific calculator.

<sup>\*</sup>The analog-to-digital converter was part of an assembly, called an "AIM box", which was supplied, courtesy of Michael Schuyler.

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APPENDIX

#### QUESTIONAIRE

# OREGON STATE UNIVERSITY CHEMISTRY DEPARTMENT CORVALLIS, OREGON (503) 754-2081

To:FacultyFrom:Stephen HawkesSubject:Significant Figure Survey

Date: March 7, 1983

To help us with a paper for J. Chem. Educ. would you please circle what you consider the correct answer to the following question:

Problem: Round the answer to the multiplication 1.43 X 4.098 = 5.86014 to the correct number of significant figures.

- (a) 6 (b) 5.9 (c) 5.86
- (d) 5.860 (e) 5.8601
- (f) The question has no unique answer (Explain):

### EIGHT CODE PROGRAMS FOR THE HP15C SCIENTIFIC CALCULATOR

The instructions for using these programs are very similar to those for the DCB routines, and do not need to be repeated in great detail.

Eight Code Mantissa Translation Program.

1 f LBL D 2 f FIX 0 3 f CLEAR REG Handling boundary condition where the sign is negative 4 ENTER 5 g ABS 6 ÷ 7 STO 3 8 q LST X 9 STO 0 R<sub>n</sub>←coded mantissa Calculation raw mod value. 10 8 11 ÷ 12 f FRAC 13 8 14 X Misc. 15 STO-0 R<sub>n</sub>←rounded value 16 g ABS 17 STO I RI←mod value 18 GTO I Go to part of program, corresponding to mod value. Mod value = 0; category of highest uncertainty. 19 f LBL 0 20 6 21 . 22 5 23 STO 1 24 3

```
25 STO 2
26 GTO 8
Mod value = 1; second-highest uncertainty category.
27 f LBL 1
28 7
29 .
30 5
31 STO 1
32 1
33 STO 2
34 GTO 8
Mod value = 2.
35 f LBL 2
36 2
37 STO-0
38 GTO 9
Mod value = 3
39 f LBL 3
40 2
41 STO+0
Third-highest uncertainty category.
42 f LBL 9
43 7
44 STO 1
45 GTO 8
Mod value = 4
46 f LBL 4
47 3
48 STO-0
49 GTO .0
Mod value = 5
50 f LBL 5
51 1
52 STO-0
53 GTO .0
Mod value = 6
54 f LBL 6
55 1
56 STO+0
```

57 GTO .0 Mod value = 7 58 f LBL 7 59 3 60 STO+0 Category of lowest 61 f LBL .0 62 5 63 STO 1 Upgestainty Calculation	-			
Uncertainty Calcula				
64 fLBL 8 65 2	X Register 2	Y Register	Z Register	T Register
66 RCL 1	R <sub>1</sub>	2		
67 2	2	R <sub>1</sub>	2	
68 ÷	R <sub>1</sub> /2	2	2	
69 YX	$_{2}R_{1}/2$	2		
70 5	5	2R1/2		
71 RCL 2	- R <sub>2</sub>	5	2R1/2	
72 4	4	R <sub>2</sub>	5	2R1/2
73 ÷	R <sub>2</sub> /4	5	2R1/2	
74 Y <sup>X</sup>	5R2/4	2R1/2		
75 X	Product			
76 RCL 0	X	Unc		
77 ÷	Únc∕ [x]			
78 gLSTX		Rel unc		
79 RCL 3	Śign	X	Unc/x	
80 X	x	Relunc		
81 g RTN				

The mean is in the  ${\sf X}$  register, and the estimated relative uncertainty is in the  ${\sf Y}$  register.

.

1 f LBL C N Preliminaries  $2 q \overline{X}$ X Register 1 contains the mean. 3 STO 1 4 1 1  $\overline{\mathbf{X}}$ 5 STO I 1 X 6 0 0 7 STO 8 Calculate the standard error of the mean and store in Register 0. 8 g s S 9 RCL 2 N S √N 10 √x S s/√N 11 ÷ 12 STO 0 If unc < 4 then scale up. s/√N 13 4 4 s/√N 4 14 x**≓**u 15 g TEST 9 (x ≥ y) 16 GTO .1  $4\sqrt{N/s}$ 17 ÷ log  $4\sqrt{N/s}$ 18 g LOG log 4√N/s 19 1 1 20 + Sum 21 g INT INT (sum) 22 STO-8 Scale count 23 10× Scale factor 24 STO X 0 25 STO X 1 26 GTO .2 If unc  $\geq$  40 then scale down. 27 f LBL .1 s/√N 4 0 28 4 s/√N 29 0 40 4 30 g TEST 7 (x>y) 31 GTO .2 s/40√N 32 ÷ 4 0

33 g LOG 34 1 35 + 36 g INT 37 CHS 38 STO-8	log s/40√N 1 Sum INT (Sum) -INT (Sum) Scale count	4 log s∕40√N	0
39 10 <sup>×</sup> 40 STO X 0	Scale factor		
41 STO X 1			
Misc.			
42 f LBL .2	_		
43 g <del>x</del>	×		
44 ENTER 45 g ABS			
46 ÷			
47 STO I			
48 g LST X			
49 STO 1	-	ontains the me	an.
50 RCL 8 51 CHS	Scale count		
52 10×	-50210 00010 10-50		
Round to the neares			
	10-SC x		
54 ENTER	10-SC x		
55 ENTER		10-SC x	10-SC x
56 8	8	10-SC x	
57 ÷	10-SC x/8	10-SC x	
58.			
59 5	.5	10-SC x/8	10-SC x
60 +	Sum	10-SC x	
61 g INT	Trunc	10-SC x	
62 8	8	Trunc	10-SC x
63 X	8 Trunc	10-SC x	
64 STO 9	-	ontains the rou	nded adjusted <del>x.</del>
How close is the ro	•		
65 - 66 STO 0	Difference Bogistor 0 c	ontains the re-	unding loca(+) or asis()
66 STO .0	negister .0 C		unding loss(+) or gain(-).

If  $Um \ge 8$  then skip ahead to the next higher uncertainty category. 67 RCL 0 Unc Dif 68 8 8 Unc Dif 69 g x <u>≤</u> y 70 GTO .3 Find correct add-on component (mod value) in the smallest uncertainty category. 71 RCL .0 Dif 8 Unc Dif 72 2 2 Dif 8 Unc 73 GSB A If yes then use (incrementing) Subroutine A. 74 CHS Dif -2 75 GSB A 76 2 4 -2 Dif 77 STO+9 If Unc  $\geq$  16 then jump ahead to next higher uncertainty category. 78 f LBL .3 79 RCL 0 Unc 80 1 81 6 16 Unc 82 g x <u>≤</u> y 83 GTO .4 Find code for the two smallest uncertainty categories. 84 RCL .0 Dif 16 85 0 0 Dif 86 GSB A 87 1 88 STO+9

Find code for the two largest uncertainty categories. 89 f LBL .4 90 2 91 5 92. 93 3 25.3 94 RCL 0 Unc 25.3 95 GSB A 96 RCL 8 97 RCL 9 . 98 RCL X I 99 f FIX 0 100 g RTN Subroutine A. Increment add-on counter if  $x \le y$ . n (or Unc) 101 fLBLA Dif (or 25.3) 102 g TEST 7 Is Dif (or 25.3) < n (or Unc)? 103 g RTN If yes, then return to calling program. Otherwise... 104 1 105 STO+9 106 RJ 107 g RTN

The integerized Eight Code mantissa is in the X register, and the ten's exponent is in the Y register.

# **COMPUTER TAPES**

Computer tapes for the DCB experiment are listed below. Included are

- 1) the experimental results for two runs
- 2) the BASIC program for interfacing the digital output of an Orion 701A lonalyzer with an AIM 65 microcomputer, and for expressing the mean and its standard error of a series of pH measurements as a single DCB number
- 3) an assembly language subroutine for reproducibly recognizing when practical equilibrium has been attained (on the next page).

EUN -9/14/84 UNCY GE Bete-1 3.052 RUN UNC? 01 36523-1 MA 3.450 LIST 110 PIKE 64 21 120 POKE 65,25 178 DEMESTRIAN 130 DEM=258 130 Derejsa er 140 Feb: I=1: D=10 150 H=16 E=4031 160 D1M BKI 170 FER I=1 TO I 180 R=FEER (1+1) 190 NE=INT (F (H) 200 02==-H+42 210 Bile=D-N1+N2 220 NEE 230 DATH. 80801\*B(1) +.081+8(2)+.1\* 235 DRT=DRT+25/4 240 INPUT "UNC"; UNC 250 IF UNCO4 GOTC30 Ø 260 UNC=D\*UNC 270 DAT=D\*DAT 280 F=F-1

290 6070250 300 IF Uncle40 Goto 340 310 F=F+1 316 FFFF1 728 UN(F1N0/E 310 UFTF1AT/D 140 P1F0 150 IFT1N1(FEME(SEC \*10\*102 I US0T0380 360 R(FF1+1 370 3070150 330 HR=EXPIRE\*LOG(2  $\langle \cdot \rangle$ 290 T=1-7 2\*HR) 400 REDATHEAHRAINT(  $\mathbf{T}$  ) 410 IF RG=HR G0T043 8 420 DET=E\*HRAINT(T) +∃⊮HP 425 0070440 430 DAT=2\*HE\*INT(T) +HR 440 SF=LE0(STR≢(DAT ))**-**1 |460 D#=STR\$(DAT) |470 PRINT " ";D\$;"E \*:1-5= \*,1-55

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The next 1.6 pages are a listing of the BASIC program for interfacing a Perkin-Elmer LC-55 spectrophotometer with an AIM 65 microcomputer, and for expressing the mean and its standard error for a series of measurements into a single Eight Code number. After that, the results for several runs of the Eight Code experiment are listed.

8/11/84 01001.= Nel: 1157 1 REM 100%3 PROGRAM 2 REM Dom Skeleton 5-610 3 PRIME ILM1/ABSOR BANCE= > A INFLIGET PRINTIRA 5 DIMARIES (100) 10 8=40390 4±14 M=2 32:0=16 11 V=258 20 FOKE8-1 0(POKE8+ 20 FUNEBF1 FINKEB+ 3/255 PINEB+11,64 25 FONEBF1- 192:POK E41334 111 FONEB+12, 224 FONEBF4 78 23 FCF1=MTCM+P:READ A:POME1 + NEMT \_29 D=.133/2740/2048 ) 30 INF.TH: 04TA POI NTS" N 12 PRINTANALAN 15 IFN(101-ADN)160T 048 35 FRINT STHE NUMBE R GF DATA FROMME NINTE TIET EE FROM" D7 FPIAT (1 TO 100" (GCT030 40 Figrestore 75 ifts athemprints "INTERVAL MUST BE AT PRINTELEAST 0.2 S ECONDERIGIT 150 PRINT'HIT SPACE TO BEGINE 200 FOFI=1TON 210 IFF=130T0218 216 GETE# IFA#<>" " G0T0215 218 IFI=2THENPOKEB+ 5,195: POKE252, 2: POKE 253, 0: POKE254, 0

RODNAEL, FIM 65

220 J=PEEK(253)+V\*P EEK(254) 240 JFJ(71+(1-1)\*FG 010220 245 7(2)=3 250 POKEB+1,1 260 POREE+12, 192: PO KEB+12, 224 310 L=PEEK(B):POKEB +1,9;H=PEEK(E) 320 A(1)=L\*U+H/U+0 330 PRINTE A(I)/D/" MV<sup>™</sup> 390 NEXT 440 7=0.3=0 500 FORI-1TON: S=S+A (I):T=T+E(1)\*A(1) 511 NEXT 515 AV=3.425 520 PB1N7(PPC MV=\*) AV 525 W=KT/D/D-N+8V+8 ₩>/(№-1) 530 PRINT "SD="; SOR (W): \*MC\* 540 0010700 600 DATA72,173,4,16 0,198,252,208,10,169 2 610 DPTA103,252,230 3253,268,2,236,254,<u>1</u> 04,64 700 PER IGRVERT MY TOCONC 710 TR=80/3608 720 STR=SQF(W)/8000 730 AB=-L0G(TR)/L0G  $\langle 10 \rangle$ 740 DAB=-106(TR+STR )/106(10) 750 SAB=AB3(AB-DAB) 760 DAT=924RAT 770 UNC=SAB\*RAT 780 PRINT "CONC=";D AT: "+-": UNC 790 REM ADJUST UNC 800 F=0 810 JFUNC2460T0860 820 UNC=10+UNC 830 DAT=10+DAT 840 F=F-4 850 0070810 860 IFUNC(486070910 870 UNC=UNC/10

CONCURSECREENCE: 1 N= 3 2223.61809 MV 2829.14570 MV 2409.54774 MV AV MV= 2820 77052 SD= 407.0598 MV CONC= .451722231 +-.0585482125

52 E-2

4452 28121 MV 4040 20101 MV 3636 19895 MV AV MV= 4042.55109 SD= 401 045505 MV CONC= 296327052 +-0416551988

36 E-2 55-50-45

T/8+.5: 930 AD=0 940 IFUNCD16+SOR(2) 50G0T01140 950 IFUNC(1680T0980 960 AD=1 970 GCT01140 980 IFUNC(860T01040 990 IFDF>000T01020 1000 AD=1 1010 60701140 1020 AD=0 1030 G0701240 1040 IFDF0-26070107 Ð 1058 AD=4 1000 HDF4 1060 GCT01140 1070 IFDF0000T01100 1080 ADF5 1090 GDT01140 1100 IFDF0100T01130 1110 -£;=∂ 1128 50701140 1138 65=7 1148 FRINT(\* \*)\* \* 1150 FRINT( DAT-DF+ AD: "E": F 1160 PRINTER PEPRIN

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680 DAT=DAT/10

900 CCT0860 910 REM CCDING

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890 F=F+1

CONC/RESCREAMCE= 2.311 N= 3 7535.17588 MV 7258 28141 MV 6831.55813 MV AV MV= 7207 7052 5D= 254 26542 MV CONC= .104672058 +-.0481565491 15 3-1 96-90-85 N= 3

500 nm

CONC.'RESCREPHICE=

4188 44111 ™√

4166 49111 MV 4040 20101 MV 2078,53441 MV AV MV= 4005 17588 SD= 155 319659 MV CONC= 1297117518 +-.0164563019

1 N= 3

297 E-J

52-50-4-8

CONC / RESIDENCE = 1 N= 3 . 4025.11563 MV 3925 64324 MV 4056.25128 MV AV MV= 4001.67504 SD= 63.6295615 MV CONC= .308848168 +-6.85127289E+03 308 E-3 50-50-50

4273.86535 MM 3939.69849 MV 3783.9195 MV AV MV= 3995.16248 SD= 258 229127 MV CONC= 301120938 +-.0253675265 104 E-3 CONC.'HEBCREHNDE= 1 1 3 43/50/57 3473.8335 4 4050.25126 MV 4050.25126 MV 4515 07523 MV AV MV= 4025.07538 SD= 518 401520 MV CONC= .255355284 +-.0527455705 R4 F41 36 E-2

CONC/ABSORBANCE=

N= 3 53-50-47

1

CONC/REFIRENCE= 1 N= 3 60-50-.40 N= 3 4V 20 - TO 4753 TAIAT MY 4025.12581 M 3221.10550 MY AV NV= 4001 67504 SD= 763 112407 MY CONC= .200848168 +-.0762482491 37 F-2 37 E-2

97

CONC/ABSORBANCE= 1 N= 3 2845 72357 MV 4036.15675 MV 5182.41769 MV AV MV=-4828.1005 SD= 1168.37413 MV CONC= .238853075 +-.110802787 34 E-2

CONC/RESORBENCE= 1 N= 3 5648.24121 MV 4005.02513 MV 2432.1608 MV AV MV= 4028.47571 SD= 1608.16844 MV CONC= .257349237 +-.145879359 34 E-2

CONC/ABSORBANCE= 1 N= 3 3630.65327 MV 4020 1035 NV 4349 24523 MV AV MV= 4000 SD= 359.717931 MV CONC= .301029395 +-.0373984 304 E-3 CONC/ABSORBANCE= 1 56-50-44 N= 3 4515.07538 MV 4045.22513 MV 3572.86433 MV AV MV= 4044.38861 SD= 471.1061 MV CONC= .295237108 +-.047852459 36 E-2

CONC/ABSORBANCE= 1 N= 3 3648.24121 MV 4037.68844 MV 4329.14573 MV AV MV= 4005 02513 SD= 341.625397 MV CONC= .300484742 +-.0355494787 304 E-3

98