Intrumentation for Characterization of Nanomaterials (v11)

Significant Figures and Round-Off Criteria for Numerical Expressions

Numerical expressions that represent the results of actual or simulated measurements should be conveyed using appropriate *significant figure*s (SFs), to preserve the accuracy with which an actual (or hypothetical) resulting, calculated quantity is known. SFs are a notational device that imply an underlying appreciation for error propagation, in cases where more explicit expressions of the associated errors and their corresponding analysis is overly cumbersome or unnecessary. For example, the expression $L = 24.3$ cm can be inferred to represent $L = (24.30 \pm 0.05)$ cm, or $L = 24.30(5)$ cm.

Significant Figures

The number of SFs in an expression is given by the total number of digits, counting from the highest-order (left-most, non-zero) digit towards lower-order positions (i.e., to the right). This includes trailing zeros to the right of the decimal point (the fractional portion of the expression). However, if the expression contains no decimal point, trailing zeros are ambiguous, and are typically not considered SFs.

When counting the number of SFs, the highest-order digit included in the sum must not be "0" or "1". Why is this? Consider, for example, the expressions $t_1 = 1.5$ s and $t_2 = 8.5$ s. For t_1, the second digit ("5") represents $0.5/1 = 50$ % of the first digit ("1"); for t_2, the "5" represents only $0.5/8 = 6\%$ of the "8". In this case, t_1 was expressed with one SF; t_2 was expressed with two SFs. Note that expressions such as 1, 10, and 10^6 essentially represent orders of magnitude, with no SFs.

Think of it this way: For the sake of discussion, let's say that if a quantity has one SF, we would roughly expect to know its value within a range of about $0.1^1 = 10\%$ of the best estimate. For two SFs, the range is about $0.1^2 = 1\%$. We could write the quantities above as $t_1 = (1.50 \pm 0.05)$ s and $t_2 = (8.50 \pm 0.05)$ s. We have 1.45 s $\leq t_1 < 1.55$ s and $0.10/1.50 = 6.7\%$, which rounds up to 10%, or one SF. But 8.45 s $\leq t_2 < 8.55$ s, and $0.10/8.50 = 1.2\%$, which rounds down to 1% or two SFs.

Round Off

It is usually necessary to *round off* a calculation result to convey the appropriate number of SFs. This is the process of removing figures that are not considered significant, and possibly altering the least significant figure (LSF) of the reported result. If the digit following the LSF is in the range 0 to 4, the LSF is unchanged; if the digit following the LSF is in the range 5-9, the LSF is increased by 1, in which case, if the LSF is a 9, the higher SFs may be affected.

Examples: Various ways to express π ($\pi = 3.14159265...$):

    1 SF: $\pi = 3$

    2 SF: $\pi = 3.1$

    5 SF: $\pi = 3.1416$ //The LSF was rounded up because the digit immediately to its right is a "9".

    6 SF: $\pi = 3.14159$

It is important to avoid ambiguity in the number of SFs when expressing a quantity. For example, consider the expression:

    $L = 240$ mm

The number of SFs here is ambiguous, due to the trailing zero, with no SFs to the right of the decimal point. Three methods are available to remedy this ambiguity (assume the quantity is known to three SFs):

1) Use scientific notation: $L = 2.40 \times 10^2$ mm

2) Change units: $L = 24.0$ cm

3) Append a decimal point: $L = 240.$ mm

Method

If we compute a quantity y as a function of a measured quantity x, i.e. $y = f(x)$, where x has a small uncertainty δx, we can usually find δy using 1st-order error analysis:

$$\delta y = \left| \frac{df}{dx} \right| \cdot \delta x$$

If the quantity depends on multiple, independent variables, say $y = f(x_1, x_2, ...)$, we can compute the uncertainty contributions from each of these:

$$\delta y_i = \left| \frac{\partial f}{\partial x_i} \right| \cdot \delta x_i$$

The combined uncertainty is estimated by adding in "quadrature":

$$\delta y = \sqrt{(\delta y_1)^2 + (\delta y_2)^2 + ...}$$

Sometimes, however, the 1st-order error is smaller than higher-order terms. A Taylor's expansion in each variable gives

$$\delta y_i = \left| \sum_{n=1}^{\infty} \left(\frac{1}{n!} \frac{d^n f}{dx_i^n} \right) \cdot \delta x_i^n \right|$$

If the 1st order term is small, the 2nd order term may dominate:

$$\delta y_i = \left| \left(\frac{\partial f}{\partial x_i} \right) \cdot \delta x_i + \frac{1}{2} \cdot \left(\frac{d^2 f}{dx^2} \right) \cdot \delta x_i^2 \right|$$

Error propagation rules can be used to determine the proper number of SFs with which to measure the result of a calculation.

Calculation results may require *round off* to convey the appropriate number of SFs. This does *not* mean that values fed into calculations should be rounded-off, nor that the full precision of the calculation should not be recorded, only that expression of the final calculation results may require round off to the appropriate number of SFs.

Multiplication & Division

The number of SFs in a result is equal to the number of SFs in the factor, quotient, or divisor with the smallest number of SFs

Example: Compute a velocity from measured distance and time:

$d = 72.6$ cm (3 SFs), $t = 8.2$ s (2 SFs)

$$v = \frac{d}{t} = \frac{72.6 \text{ cm}}{8.2 \text{ s}} (= 8.8537... \text{ cm/s}) = \underline{\underline{8.9 \text{ cm/s}}} \text{ (2 SFs)}$$

Addition & Subtraction

The number of SFs in the addends, minuend, or subtrahend do not directly affect the number of SFs in the results. Rather, the LSF of of the results should be in the same position as the LSF of the term(s) having its LSF furthest to the left.

Example: Compute a total length from two segments measured with different methods:

$L_1 = 209.0$ nm , $L_2 = 1.822$ nm (3 SFs)

$L = L_1 + L_2 = 209.0 \text{ nm} + 1.822 \text{ nm} (= 210.822 \text{ nm}) = \underline{\underline{210.8 \text{ nm}}} \text{ } (10^{-1} \text{ LSF})$

Exponents

For a base raised to an exponent (without error), the number of SFs decreases slowly as the absolute value of the exponent is increased above "1" (when the base and result are equal and have the same number of SFs), decreasing by approximately one for an exponent of "10". For fractional exponents, the number of SFs actually increases slightly. The result of raising a base to an exponent of "0.1" actually adds approximately one SF, compared to the base value. The reciprocal of a number has the same number of SFs as the original.

Example: Compute the area of a circle from a measured diameter:

$D = 1.506$ μm (3 SFs)

$$A = \frac{\pi}{4} \cdot D^2 = \frac{3.14159...}{4} \cdot (1.506 \text{ μm})^2 (= 1.78013... \text{ μm}^2) = \underline{\underline{1.780 \text{ μm}^2}} \text{ (3 SFs)}$$

Example: Compute the volume of a 10-D hypercube from a measured edge length:

$L = 9.306$ m (4 SFs)

$V_h = L^{10} (= 4.8711... \times 10^9 \text{ m}^{10}) = \underline{\underline{4.87 \times 10^9 \text{ m}^{10}}} \text{ (3 SFs)}$

Trigonometric functions

These have somewhat different rules. For small angles, the result of the sine operation has the same SFs as the operand. But, the result of cosine for small angles generally has more SFs than the the operand. Also note that angles must be expressed in radians for correct error propagation.

Example: Compute the sine of a small angle:

$\theta = 0.40°$ (2 SFs)

$y = \sin \theta (= 0.00698126...) = \underline{\underline{0.0070}}$ (2 SFs)

Example: Compute the cosine of the same small angle:

$\theta = 0.40°$ (2 SFs)

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We may consider this to imply $\theta = 0.400° \pm 0.005°$. Computationally

$$y + \delta y = \cos(\theta + \delta\theta)(= 0.99997502...)$$

$$y - \delta y = \cos(\theta - \delta\theta)(= 0.99997624...)$$

$$\delta y = |[\cos(\theta + \delta\theta) - \cos(\theta - \delta\theta)]/2|(= 0.000000613...)$$

Note that angles must be converted to radians for correct error propagation. The uncertainty is in the sixth digit after the decimal place

$$y = \cos\theta(= 0.99997563...) = \underline{0.999976} \ (6 \text{ SFs})$$

In this case, the 1st order contribution is smaller than the 2nd order contribution. Expanding to 2nd order gives the same result as our computational estimation:

$$\delta y = \left| -\sin\theta \cdot \delta\theta - \frac{1}{2} \cdot \cos\theta \cdot \delta\theta^2 \right|(= 0.000000613...)$$

Example: The inverse cosine only requires a 1st order estimation, but the math is trickier:

$$y = 0.999976 \ (6 \text{ SFs})$$

$$\theta = \cos^{-1} y(= 0.3969576...) \ (6 \text{ SFs})$$

$$\delta\theta = \left| \frac{1}{\sqrt{1 - y^2}} \cdot \delta y \right|(= 0.00417806...°)$$

The uncertainty is in the 3rd digit after the decimal place, so

$$\theta = \underline{0.40°} \ (2 \text{ SFs})$$

Of course, we could also have $\theta = -0.40°$, but that is another discussion.