Appendix A

Common Mathematical Operations in Chemistry

In addition to basic arithmetic and algebra, four mathematical operations are used frequently in general chemistry: manipulating logarithms, using exponential notation, solving quadratic equations, and graphing data.

MANIPULATING LOGARITHMS

Meaning and Properties of Logarithms

A logarithm is an exponent. Specifically, if $x^n = A$, we can say that the logarithm to the base x of the number A is n, and we can denote it as

$$\log_{x} A = n$$

Because logarithms are exponents, they have the following properties:

$$\log_x 1 = 0$$

$$\log_x (A \times B) = \log_x A + \log_x B$$

$$\log_x \frac{A}{B} = \log_x A - \log_x B$$

$$\log_x A^y = y \log_x A$$

Types of Logarithms

Common and natural logarithms are used in chemistry and the other sciences.

1. For *common* logarithms, the base (x in the examples above) is 10, but they are written without specifying the base. That is, $\log_{10} A$ is written more simply as $\log A$; thus, the notation $\log A$ means base 10. The common logarithm of 1000 is 3; in other words, you must raise 10 to the 3rd power to obtain 1000:

$$\log 1000 = 3$$
 or $10^3 = 1000$

Similarly, we have

$$\log 10 = 1$$
 or $10^1 = 10$
 $\log 1,000,000 = 6$ or $10^6 = 1,000,000$
 $\log 0.001 = -3$ or $10^{-3} = 0.001$
 $\log 853 = 2.931$ or $10^{2.931} = 853$

The last example illustrates an important point about significant figures with all logarithms: *the number of significant figures* in the number equals the number of digits to the right of the decimal point in the logarithm. That is, the number 853 has three significant figures, and the logarithm 2.931 has three digits to the right of the decimal point.

To find a common logarithm with an electronic calculator, enter the number and press the LOG button.

2. For *natural* logarithms, the base is the number e, which is 2.71828 ..., and $\log_e A$ is written $\ln A$; thus, the notation $\ln A$ means base e. The relationship between the common and natural logarithms is easily obtained:

$$\log 10 = 1$$
 and $\ln 10 = 2.303$

Therefore, we have

$$\ln A = 2.303 \log A$$

To find a natural logarithm with an electronic calculator, enter the number and press the LN button. If your calculator does not have an ln button, enter the number, press the LOG button, and multiply by 2.303.

Antilogarithms

The *antilogarithm* is the base raised to the logarithm:

antilogarithm (antilog) of
$$n$$
 is 10^n

Using two of the earlier examples, the antilog of 3 is 1000, and the antilog of 2.931 is 853. To obtain the antilog with a calculator, enter the number and press the 10^x button. Similarly, to obtain the natural antilogarithm, enter the number and press the e^x button. [On some calculators, you need to enter the number and first press inv and then the log (or ln) button.]

USING EXPONENTIAL (SCIENTIFIC) NOTATION

Many quantities in chemistry are very large or very small. For example, in the conventional way of writing numbers, the number of gold atoms in 1 gram of gold is

59,060,000,000,000,000,000,000 atoms (to four significant figures)

As another example, the mass in grams of one gold atom is

0.00000000000000000000003272 g (to four significant figures)

Exponential (scientific) notation provides a much more practical way of writing such numbers. In exponential notation, we express numbers in the form

$$A \times 10^n$$

where A (the coefficient) is greater than or equal to 1 and less than 10 (that is, $1 \le A <$, 10), and n (the exponent) is an integer.

If the number we want to express in exponential notation is larger than 1, the exponent is positive (n > 0); if the number is smaller than 1, the exponent is negative (n < 0). The size of n tells the number of places the decimal point (in conventional notation) must be moved to obtain a coefficient A greater than or equal to 1 and less than 10 (in exponential notation). In exponential notation, 1 gram of gold contains 5.906×10^{22} atoms, and each gold atom has a mass of 3.272×10^{-22} g.

Changing Between Conventional and Exponential Notation

In order to use exponential notation, you must be able to convert to it from conventional notation, and vice versa.

1. To change a number from conventional to exponential notation, move the decimal point to the left for numbers equal to or greater than 10 and to the right for numbers between 0 and 1:

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75,000,000 changes to 7.5 \times 10^7 (decimal point 7 places to the left) 0.006042 changes to 6.042 \times 10^{-3} (decimal point 3 places to the right)
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2. To change a number from exponential to conventional notation, move the decimal point the number of places indicated by the exponent to the right for numbers with positive exponents and to the left for numbers with negative exponents:

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1.38\times10^5 changes to 138,000 (decimal point 5 places to the right) 8.41\times10^{-6} changes to 0.00000841 (decimal point 6 places to the left)
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3. An exponential number with a coefficient greater than 10 or less than 1 can be changed to the standard exponential form by converting the coefficient to the standard form and adding the exponents:

$$582.3 \times 10^6$$
 changes to $5.823 \times 10^2 \times 10^6 = 5.823 \times 10^{(2+6)} = 5.823 \times 10^8$
 0.0043×10^{-4} changes to $4.3 \times 10^{-3} \times 10^{-4} = 4.3 \times 10^{((-3)+(-4))} = 4.3 \times 10^{-7}$

Using Exponential Notation in Calculations

In calculations, you can treat the coefficient and exponents separately and apply the properties of exponents (see earlier section on logarithms).

1. To multiply exponential numbers, multiply the coefficients, add the exponents, and reconstruct the number in standard exponential notation:

$$(5.5 \times 10^{3})(3.1 \times 10^{5}) = (5.5 \times 3.1) \times 10^{(3+5)} = 17 \times 10^{8} = 1.7 \times 10^{9}$$

 $(9.7 \times 10^{14})(4.3 \times 10^{-20}) = (9.7 \times 4.3) \times 10^{[14+(-20)]} = 42 \times 10^{-6} = 4.2 \times 10^{-5}$

2. To divide exponential numbers, divide the coefficients, subtract the exponents, and reconstruct the number in standard exponential notation:

$$\frac{2.6 \times 10^6}{5.8 \times 10^2} = \frac{2.6}{5.8} \times 10^{(6-2)} = 0.45 \times 10^4 = 4.5 \times 10^3$$
$$\frac{1.7 \times 10^{-5}}{8.2 \times 10^{-8}} = \frac{1.7}{8.2} \times 10^{[(-5)-(-8)]} = 0.21 \times 10^3 = 2.1 \times 10^2$$

3. To add or subtract exponential numbers, change all numbers so that they have the same exponent, then add or subtract the coefficients:

$$(1.45\times10^4) + (3.2\times10^3) = (1.45\times10^4) + (0.32\times10^4) = 1.77\times10^4$$

 $(3.22\times10^5) - (9.02\times10^4) = (3.22\times10^5) - (0.902\times10^5) = 2.32\times10^5$

SOLVING QUADRATIC EQUATIONS

A quadratic equation is one in which the highest power of x is 2. The general form of a quadratic equation is

$$ax^2 + bx + c = 0$$

where *a*, *b*, and *c* are numbers. For given values of *a*, *b*, and *c*, the values of *x* that satisfy the equation are called *solutions* of the equation. We calculate *x* with the quadratic formula:

$$x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

We commonly require the quadratic formula when solving for some concentration in an equilibrium problem. For example, we might have an expression that is rearranged into the quadratic equation

$$4.3x^2 + 0.65x - 8.7 = 0$$

Applying the quadratic formula, with a = 4.3, b = 0.65, and c = -8.7, gives

$$x = \frac{-0.65 \pm \sqrt{(0.65)^2 - 4(4.3)(-8.7)}}{2(4.3)}$$

The "plus or minus" sign (\pm) indicates that there are always two possible values for x. In this case, they are

$$x = 1.3$$
 and $x = -1.5$

In any real physical system, however, only one of the values will have any meaning. For example, if x were $[H_3O^+]$, the negative value would give a negative concentration, which has no physical meaning.

GRAPHING DATA IN THE FORM OF A STRAIGHT LINE

Visualizing changes in variables by means of a graph is used throughout science. In many cases, it is most useful if the data can be graphed in the form of a straight line. Any equation will appear as a straight line if it has, or can be rearranged to have, the following general form:

$$y = mx + b$$

where y is the dependent variable (typically plotted along the vertical axis), x is the independent variable (typically plotted along the horizontal axis), m is the slope of the line, and b is the intercept of the line on the y axis. The intercept is the value of y when x = 0:

$$y = m(0) + b = b$$

The slope of the line is the change in y for a given change in x:

Slope (m) =
$$\frac{y_2 - y_1}{x_2 - x_1} = \frac{\Delta y}{\Delta x}$$

The sign of the slope tells the direction of the line. If y increases as x increases, m is positive, and the line slopes upward with higher values of x; if y decreases as x increases, m is negative, and the line slopes downward with higher values of x. The magnitude of the slope indicates the steepness of the line. A line with m=3 is three times as steep (y changes three times as much for a given change in x) as a line with m=1.

Consider the linear equation y = 2x + 1. A graph of this equation is shown in Figure A.1. In practice, you can find the slope by drawing a right triangle to the line, using the line as the hypotenuse. Then, one leg gives Δy , and the other gives Δx . In the figure, $\Delta y = 8$ and $\Delta x = 4$.

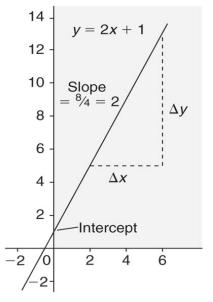


Figure A.1

At several places in the text, an equation is rearranged into the form of a straight line in order to determine information from the slope and/or the intercept. For example, in Chapter 16, we obtained the following expression:

$$\ln \frac{[A]_0}{[A]_t} = kt$$

Based on the properties of logarithms, we have

$$\ln [A]_0 - \ln [A]_t = kt$$

Rearranging into the form of an equation for a straight line gives

$$\ln [A]_t = -kt + \ln [A]_0$$
$$y = mx + b$$

Thus, a plot of $\ln [A]_t$ vs. t is a straight line, from which you can see that the slope is -k (the negative of the rate constant) and the intercept is $\ln [A]_0$ (the natural logarithm of the initial concentration of A).

At many other places in the text, linear relationships occur that were not shown in graphical terms. For example, the conversion of temperature scales in Chapter 1 can also be expressed in the form of a straight line:

$${}^{\circ}F = \frac{9}{5} {}^{\circ}C + 32$$

 $y = m x + b$