Module 1: Foundations

Mathematical Foundations

Fundamentals of Chemistry Open Course

Learning Objectives | Module 1

1. Extract useful quantitative information from problems; generate a list of known and unknown quantities from the text of a problem.
2. Solve equations for a single unknown variable using standard algebraic operations.
3. Draw and interpret graphs relating physical variables with relevance to chemistry.
4. Recognize the essential components of a measurement.
5. Apply dimensional analysis with knowns and unknowns to solve equations involving measured quantities.
6. Calculate measures of accuracy and precision to assess the quality of a set of measurements.
7. Express quantities calculated from measurements at the appropriate level of precision by applying the rules for significant digits.
8. Recognize and distinguish between physical and chemical properties.
9. Classify different types of matter as pure substances or mixtures; compare and contrast homogeneous and heterogeneous mixtures.
10. Describe and apply the scientific method.

Extracting the Knowns and Unknowns

- Quantitative problems in chemistry contain embedded **variables**.
  - **Known variables** are associated with specified values, usually in the form of measurements.
  - **Unknown variables** are assigned letters; solving for one or more unknowns is the goal of the problem.
- Reading through the problem text and extracting the known and unknown variables is a key first step when solving problems in chemistry. Doing this will often point us toward a relation between the variables!

Example. List the known and unknown variables in the problem text below.

How many moles of gaseous boron trifluoride (BF_3) are contained in a 4.3410-L bulb at 788.0 K if the pressure is 1.220 atm?

Algebra Review

- Once an appropriate equation relating the known and unknown variables is found, solving for the unknown variable is usually just a matter of algebra.

- Rearrange linear equations (with the unknown variable to the first power) using standard arithmetic operations:
  - Add a quantity to both sides
  - Subtract a quantity from both sides
  - Multiply both sides by a quantity
  - Divide both sides by a quantity

- For equations with the unknown to the n^{th} power, raise both sides to the $1/n^{th}$ power or "take the n^{th} root of both sides."

- Solve quadratic equations using the quadratic formula. Two solutions will result; usually, only one makes physical sense!

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

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

Algebra Review

- Equations containing the exponential function e^x can be solved by taking the natural logarithm of both sides. Related equations containing n^x, where n is an arbitrary number, can be solved the same way.

$$e^x = K \qquad \ln(e^x) = \ln K \qquad x = \ln K$$

$$n^x = K \qquad \ln(n^x) = \ln K \qquad x \ln n = \ln K \qquad x = \frac{\ln K}{\ln n}$$

- Looking for additional information and practice? Check out the GT Open College Algebra site.

Drawing and Interpreting Graphs

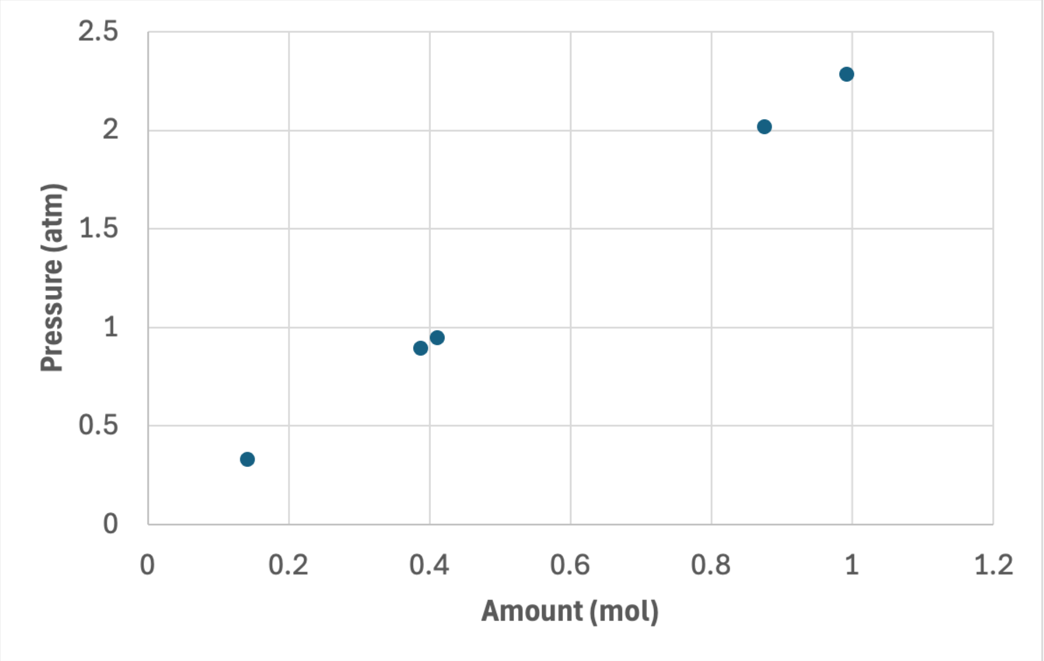
- **Graphs** depicting relations between two or more variables will appear regularly throughout your study of chemistry.

- A **scatter plot** depicts two-dimensional data as a set of points on a plane.
  - The horizontal axis (***x*-axis**) is typically used for the **independent variable**, which was varied freely when the data was collected.
  - The vertical axis (***y*-axis**) is typically used the **dependent variable**, which was measured in response to a change in the independent variable.

- Each axis is associated with a **scale** that includes specified units.

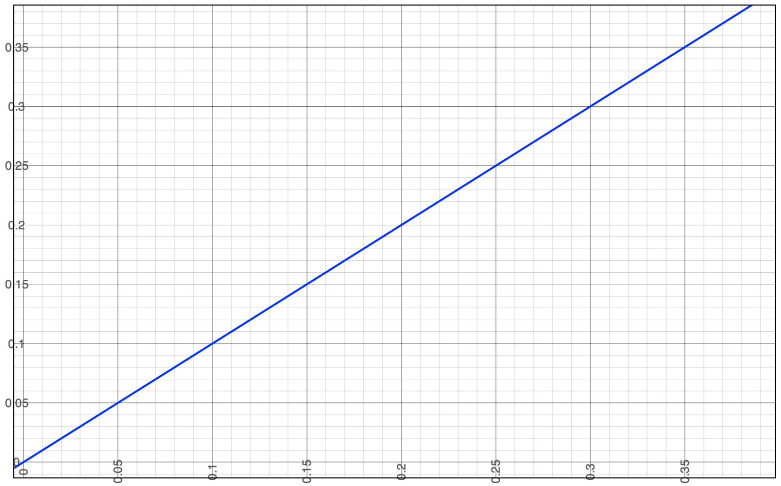
- We will most often draw graphs using spreadsheet software such as Microsoft Excel.

Amount (mol)	Pressure (atm)
0.142	0.3266
0.388	0.8924
0.412	0.9476
0.876	2.0148
0.992	2.2816

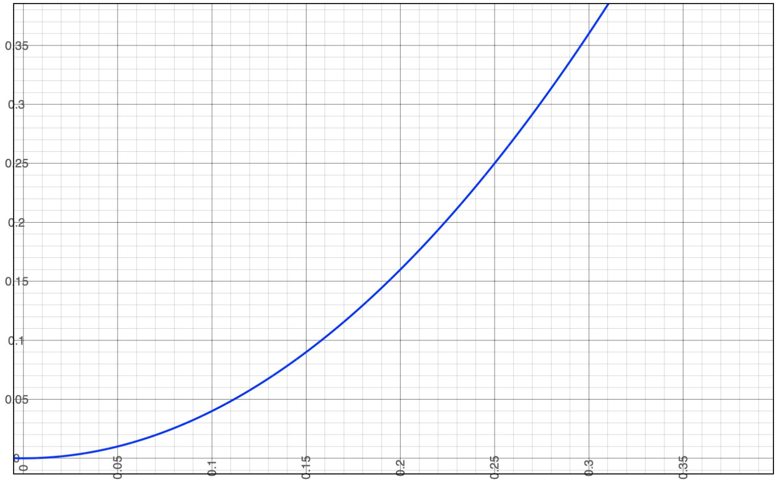


Drawing and Interpreting Graphs

- We will encounter several different types of mathematical relations between variables…
  - **Linear: $y = mx + b$.** The variable y increases at a constant rate with respect to the variable x and *vice versa*.



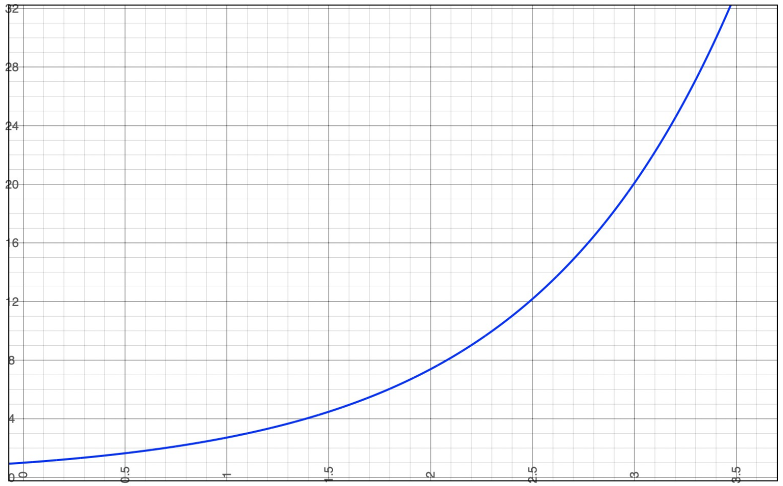
  - **Quadratic: $y = ax^2 + bx + c$.** A parabolic relation. The rate of change of y with respect to x varies linearly with x.



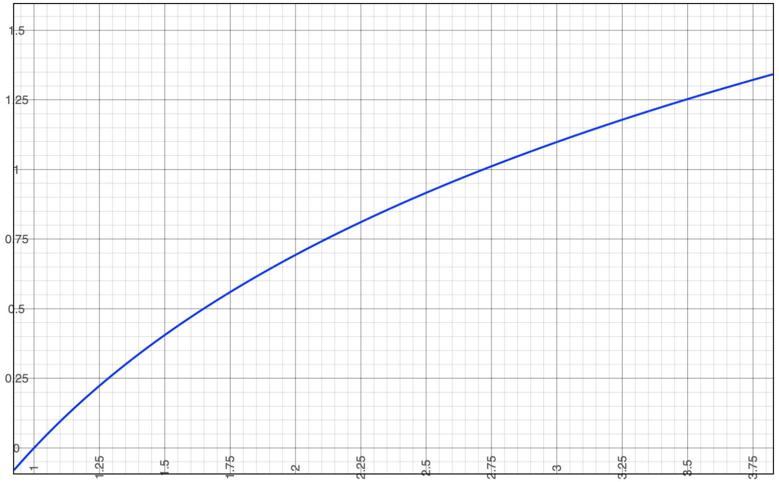
Drawing and Interpreting Graphs

- We will encounter several different types of mathematical relations between variables…

  - **Exponential: $y = ae^x$.** The variable *y* increases extremely rapidly with respect to *x*.



  - **Logarithmic: $y = a \ln x$.** The inverse of an exponential relation; *y* increases very slowly with respect to *x*.



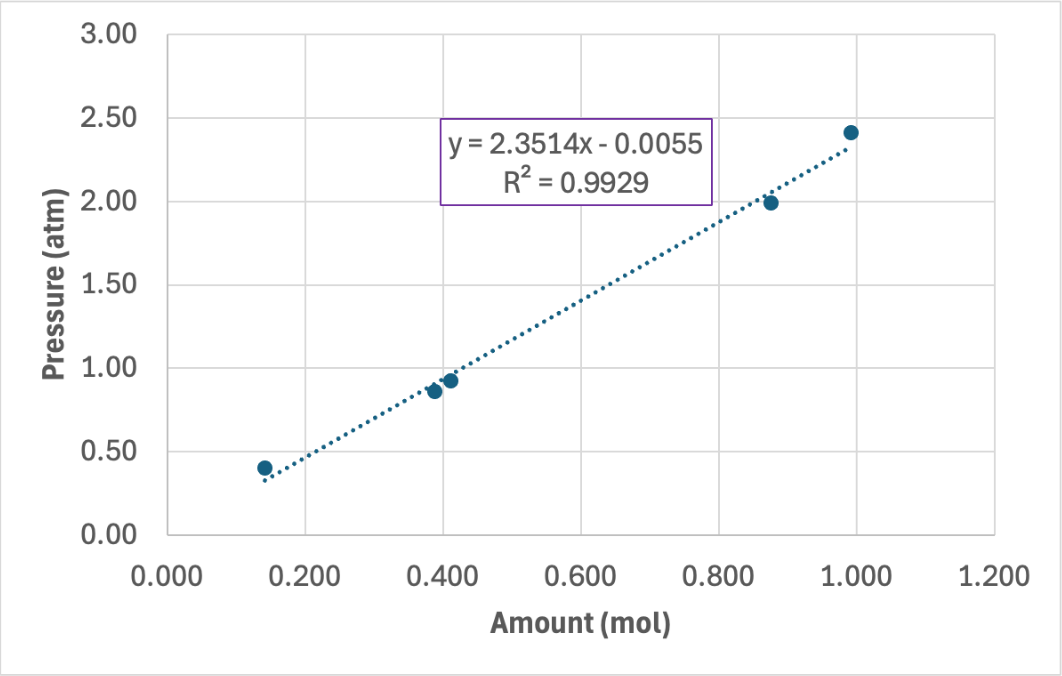
Fitting Data to a Mathematical Model

- Frequently, especially in a laboratory context, we will have an idea of a mathematical model that measured data *should* follow. Fitting the data to the model provides empirical support for the validity of the model.

- Fitting is a matter of minimizing the deviation of the modeling line or curve from the data points. Finding the optimal line through a set of points related linearly is called **linear regression**.

- Spreadsheet software will carry out linear regression for us; however we will sometimes need to transform a nonlinear relation into a linear one first (linearization; see the next slide).

Amount (mol)	Pressure (atm)
0.142	0.40
0.388	0.86
0.412	0.92
0.876	1.99
0.992	2.41



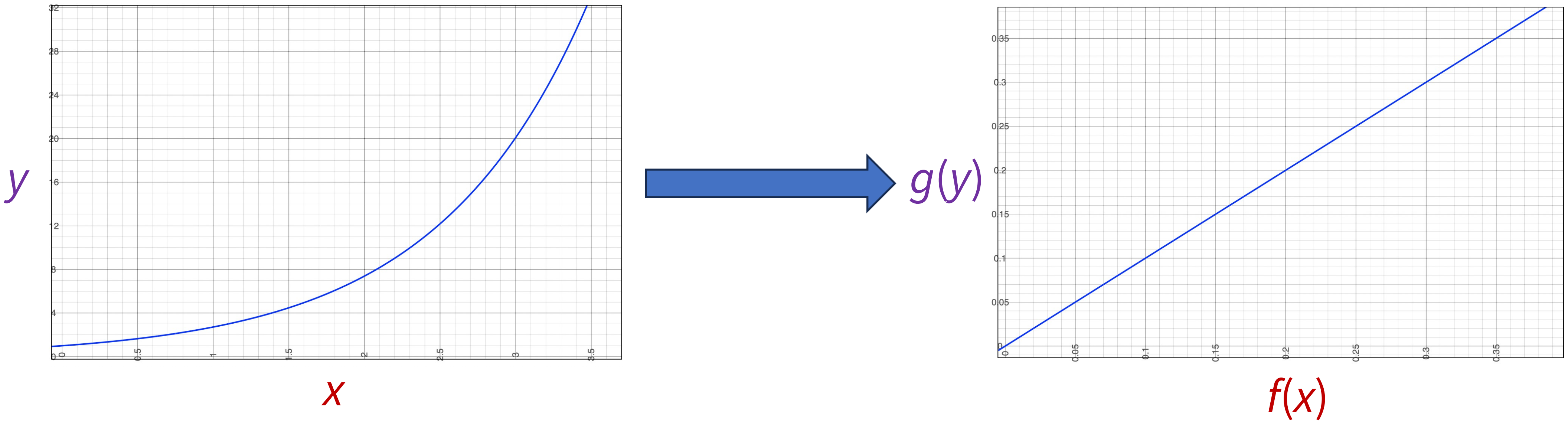
Fitting Data to a Mathematical Model

- A nonlinear graph can be converted into a linear one by plotting appropriate functions of the variables x and y. This process is called **linearization**.

- Consider two sets of data $\{x_i\}$ and $\{y_i\}$ related theoretically by the general equation…

$$g(y_i) = M \times f(x_i) + B$$

- A plot with $g(y)$ on the vertical axis and $f(x)$ on the horizontal axis will then be linear with slope M and intercept B. Linear regression can then be applied to the transformed set of data $\{f(x_i), g(y_i)\}$ to determine the best-fitting M and B.



Example. The rate constant *k* of a chemical reaction generally increases with absolute temperature *T* according to the general equation below (*A* and *B* are constants). Linearize the equation and show how a plot of the appropriate functions of *k* and *T* appears linear. Determine *A* and *B* based on the given set of data.

$$k = Ae^{-B/T}$$

Temperature (K)	**Rate constant (s^{-1})**
293	0.0011
303	0.0035
317	0.0080
323	0.0113