# EPSC 220: Principles of Geochemistry Laboratory 1: Introduction to Geochemical Calculations with MATLAB

***MATLAB learning objectives***

Learn how to use the following functions in MATLAB: help, roots and some of the various MATLAB functions that perform numerical integration. Learn how to write a loop for an iterative calculation and use a conditional statement to exit a loop when a solution is found (using Newton's Method). Practice writing matrices in MATLAB and solving coupled systems of linear equations using the MATLAB backslash operator.

***Geochemical learning objectives:***

Review calculations of ΔH, ΔS, and ΔG for simple chemical reactions. Learn some geologically important reactions and the names and formulas of some end-member mineral formulas.

***Assessment:***

The goal of this assignment is to learn. If you make a mistake we will help you redo the assignment until you understand the results and obtain the correct answers.

Please feel free to ask for help and/or look up the information on the web that you need to help solve the following problems. However, you cannot simply download or "cut and paste" a program that your find on the web.

**1.** Measure the duration of time you need to solve the following equation for x by hand and by MATLAB (read the MATLAB help files to learn how to find the roots of polynomials):

$$3x^3+2x^2+5x-37.2 = 0$$

Using MATLAB and the data on the next page write a short program to calculate the ΔH, ΔS, and ΔG of the following reaction at 1 bar, 298 K:

$$C^{diamond} \Leftrightarrow C^{graphite}$$

**2.** Integrate the following equation from 1 to 100 using both numerical methods in MATLAB (see the help to find the correct command) and analytically using integration by parts:

$$\ln(x) + 3x^2 + 2x - 5 = 0$$

Using the data on the next page calculate the ΔH, ΔS, and ΔG of the following reaction at 1 bar, 298 K using MATLAB:

$$NaAlSi_3O_8^{plagioclase} \Leftrightarrow NaAlSi_2O_6^{clinopyroxene} + SiO_2^{quartz}$$

**3.** Write your own program in MATLAB using Newton's method to find the solution of (you will have to use a simple loop in your program):

$$5\ln(x) + 6\ln(x^2)-3x + 7 = 0$$

Using MATLAB and the data on the next page write a short program to calculate the ΔH, ΔS, and ΔG at 1 bar, 298 K of the following reaction:

$$Mg_2SiO_4^{olivine}+SiO_2^{quartz} \Leftrightarrow 2\ MgSiO_3^{orthopyroxene}$$

**4.** Use MATLAB to find the solution to the following set of equations (remember that you can express these equations in matrix form):

$$2x + 4y - 7z = 0.4482643$$
$$3x + 7y + 1.5z = 31.445008$$
$$x + y - z = 2.8390049$$

Using MATLAB and the below data write a short program to calculate the ΔH, ΔS, and ΔG of the following reaction at 1 bar, 298 K:

$$CaCO_3^{aragonite} \Leftrightarrow CaCO_3^{calcite}$$

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**Thermodynamic Data for the problem set**

| Phase | Component | $\Delta H_f^o$ (kJ $mol^{-1}$) | S (J $K^{-1}$ $mol^{-1}$) |
|---|---|---|---|
| Graphite | C | 0.0 | 5.740 |
| Diamond | C | 1.85 | 2.37 |
| Albite | $NaAlSi_3O_8$ | -3921.02 | 210.04 |
| Jadeite | $NaSlSi_2O_6$ | -3011.94 | 133.47 |
| α-Quartz | $SiO_2$ | -910.65 | 41.34 |
| Olivine | $Mg_2SiO_4$ | -2175.68 | 95.19 |
| Orthopyroxene | $MgSiO_3$ | -1546.77 | 67.86 |
| Calcite | $CaCO_3$ | -1207.30 | 92.68 |
| Aragonite | $CaCO_3$ | -1207.21 | 90.21 |

all values at 1 bar, 298 K