

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:

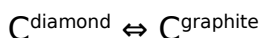
The goal of this assignment is to learn. If you make a mistake we will help you redo the assignment until you understand the results and obtain the correct answers.

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 you 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:



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:

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

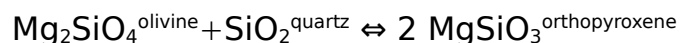
Using the data on the next page calculate the ΔH , ΔS , and ΔG of the following reaction at 1 bar, 298 K using MATLAB:



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):

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

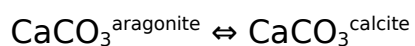
Using MATLAB and the data on the next page write a short program to calculate the ΔH , ΔS , and ΔG at 1 bar, 298 K of the following reaction:



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

$$\begin{aligned} 2x + 4y - 7z &= 0.4482643 \\ 3x + 7y + 1.5z &= 31.445008 \\ x + y - z &= 2.8390049 \end{aligned}$$

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:



Thermodynamic Data for the problem set

Phase	Component	ΔH_f° (kJ mol ⁻¹)	S (J K ⁻¹ mol ⁻¹)
Graphite	C	0.0	5.740
Diamond	C	1.85	2.37
Albite	NaAlSi ₃ O ₈	-3921.02	210.04
Jadeite	NaSiSi ₂ O ₆	-3011.94	133.47
α-Quartz	SiO ₂	-910.65	41.34
Olivine	Mg ₂ SiO 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