

EQUILIBRIUM CONSTANT

The equilibrium constant for a reaction can be roughly formulated as follows:

$$K = e^{-\frac{E}{RT}} \quad (1)$$

where E = energy barrier (calories/mole)

R = gas constant = 1.987 cal/° mole

T = temperature (Kelvin)

°C + 273.15 = Kelvin

e = natural logarithm base

1. Suppose a reaction takes place at a constant temperature of 0°C. Calculate K for the following values of E.

E, cal/mol	K
5.0	<u>0.99(1)</u>
50.	<u>0.91(2)</u>
500.	<u>0.40 (0.398)</u>
5000.	<u>1.0 x 10⁻⁴ (9.98 x 10⁻⁵)</u>
50000.	<u>9.8 x 10⁻⁴¹</u>

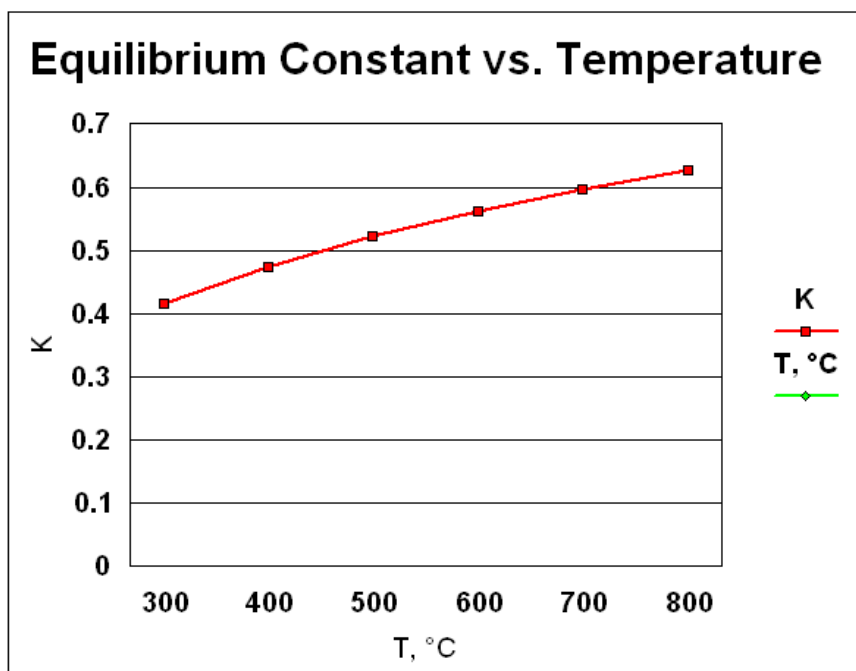
Assume all values of E are good to two significant figures.

2. Suppose a reaction takes place with a constant energy barrier of 1000 cal/mol. Calculate K for the following temperatures.

T, °C	K
300	<u>0.416 (0.4156)</u>
400	<u>0.474 (0.4735)</u>
500	<u>0.522 (0.5216)</u>
600	<u>0.562 (0.5612)</u>
700	<u>0.596 (0.5962)</u>
800	<u>0.626 (0.6257)</u>

Assume T and E values are good to three significant figures.

3. Prepare a plot of K vs. T for the temperature range 300 to 800°C. This may be done on a computer, but the plot must be printed out and handed in.



4. For a constant energy barrier of 1000 cal/mol calculate the temperature in °C at which the amount of products should equal the amount of reactants (i.e. when $K = 0.500$). This answer should be calculated to three significant figures. (HINT: Take the natural log of both sides of the above equation).

$$T = \underline{453} \text{ } ^\circ\text{C}$$

$$\ln K = \ln e^{-\frac{E}{RT}} = -\frac{E}{RT} \quad (2)$$

$$\ln 0.5 = -\frac{1000}{1.987 \cdot T} \quad (3)$$

$$T = -\frac{1000}{1.987 \cdot \ln 0.5} = -\frac{1000}{-1.377} = 726.1 \text{ } K \quad (4)$$

$$T (^\circ C) = 726.1 - 273.2 = 453 \text{ } ^\circ C \quad (5)$$