Problem set 3

Due March 24, 2026

1. Assuming thermodynamic control over the reaction of phenol nitration compute the molar fractions of *o*-nitrophenol (o) and *p*-nitrophenol (p) at $t = 80°\text{C}$ of the energy difference of these two isomers is $E_o - E_p = 1.06$ kcal/mol. Mind the degeneracy of the two isomers.

2. Derive the probability density distribution of the total velocity $v = v_x^2 + v_y^2$ where v_x and v_y are the x and y components of the velocity, of a free particle with mass m confined to a plane. Its energy is only the kinetic energy

$$E_k = \frac{1}{2}mv^2$$

   Note that the "state" described by the total velocity v is a degenerate state and its degeneracy is proportional to the perimeter of a circle with radius v. Assuming $m = 1$ D (the mass of a hydrogen atom) draw the distributions for $T = 200$ K and $T = 300$ K.

The universal gas constant $R = 8.3145$ J/(mol*K), the Boltzmann constant $k_B = R/N_A = 1.3803$ J/K, the Avogadro number, $N_A = 6.022 \times 10^{23}$, 1 kcal = 4184 J.