Homework 5 (due October 10, 2019)

(1) Barometric height distribution of gas molecules **(10 pts)**

The O_2:N_2 ratio in air is 21:78 at sea level (with the rest being mostly CO_2). This is, the concentration ratio between the two gases is $\frac{c_{O_2}}{c_{N_2}} = 0.269$.

(a) Do you expect this ratio to change or stay constant as a function of height (at constant *T*)? – Explain!

(b) Work out the O_2:N_2 ratio at a height of 8,000 m above sea level for a constant $T = 300$ K. Show the units in your calculation!

(2) The beginning of polymer statistics **(20 pts)**

We know that the two *gauche* conformations in *n*-butane have an energy $\Delta E = 0.8\ k_B T$ above that of *trans* at room temperature. Here we explore how this result can be used to describe a slightly longer *n*-alkane.

(a) Sketch a *n*-hexane molecule and discuss which bond rotations affect its conformation. Based on our statistical mechanics approach to describe the conformational variability of *n*-butane with its statistical weights w_t for *trans* and w_g for *gauche*, develop a description of the conformational variability of *n*-hexane and show that the relevant partition function can be written as $Q = w_t^3 + 6w_t^2 w_g + 12 w_t w_g^2 + 8 w_g^3$.

(b) Using the result from (a), determine the average torsional energy $\langle E \rangle$ of a sample of *n*-hexane at 300 K, assuming that the rotational states of neighboring bonds are independent and that ΔE does not change with the length of *n*-alkane chains.
What is $\langle E \rangle$ at 100 K, if you also assume that ΔE is temperature-independent, *i.e.*, ΔE = 2.0 kJ/mol (= $0.8\ k_B T$ at room temperature)?