Exercise 10

Name:	Matriculation number:
Name:	Matriculation number:

Results:

10.1	of 5 P
10.2	of 5 P
10.3	of 5 P
total	of 15 P

General instructions

- Submit your solution to Luca Donati (R. 35.17) before **Thursday 09. July at 8.15 am**.
- Fill out this cover sheet and submit it along with your solution.
- Show how you arrived at your answer.

10.1 Rotational-vibrational spectrum of $^{1}H^{127}I$ (5 P)

The absorption lines of the rotational-vibrational spectrum of $^{12}C^{16}O$ occure at the following wavenumbers

- P-Branch: 2275.90 cm^{-1}, 2263.05 cm^{-1}, 2250.20 cm^{-1}, 2237.35 cm^{-1},...
- R-Branch: 2301.60 cm^{-1}, 2314.45 cm^{-1}, 2327.30 cm^{-1}, 2340.14 cm^{-1},...

(a) Calculate the characteristic vibrational temperature Θ_{vib} and the characteristic rotational temperature Θ_{rot} of $^{1}H^{127}I$. Explain how your arrived at the results.

(b) From the characteristic vibrational temperature Θ_{vib}, calculate the ground state vibrational frequency and the bond force constant k.

(c) From the characteristic rotational temperature Θ_{rot}, calculate the moment of inertia and the bond length r.

(d) Compare your results with tabulated values for $^{1}H^{127}I$.

10.2 Mixing CO and O_2 (5 P)

Consider a container of volume $V = 0.05m^3$ which is split into two compartments with volumes $V_1 = V_2 = 0.025m^3$ by a wall. The first compartment is filled with 1 mol of ^{16}O-^{16}O. The second compartment is filled with 2 mol of ^{12}C-^{16}O. The temperature is 300 K. The characteristic temperatures for vibration and rotation of the two substances are

- ^{12}C-^{16}O: $\Theta_{vib} = 3112$ K and $\Theta_{rot} = 2.766$ K
- ^{16}O-^{16}O: $\Theta_{vib} = 2265$ K and $\Theta_{rot} = 2.068$ K

(a) Calculate the pressure in the two compartments.

(b) Calculate the free energy of mixing.

(c) Calculate the partial pressures of ^{16}O-^{16}O and of ^{12}C-^{16}O after mixing.

(d) Calculate the chemical potential of ^{16}O-^{16}O and of ^{12}C-^{16}O in the mixture.

10.3 Entropy of mixing (5 P)

Consider two gases A and B with particle numbers N_A and N_B confined to volumes V_A and V_B. These two gases are mixed in volume $V = V_A + V_B$ (analogous to exercise 10.2)

(a) Give an expression for the entropy of mixing ΔS

(b) Assume that A is the same gas as B. Given an expression for ΔS.

(c) Assume that A and B are different particles but that the particles in each gas are distinguishble. Give an expression for ΔS.