Exercise 09

Name:	Matriculation number:
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The exercise is due on Wednesday, June 27, 8 am.

9.1 Text book

If you have not done it for Exercise 08 read sections 5.1 to 5.5 and 6.1 in G.H. Findenegg, T. Hellweg „Statistische Thermodynamik"

9.2 Internal energy of an ideal gas

Calculate the internal energy of He, Ne and Ar at thermodynamic standard conditions. Is there an easy way to obtain the internal energy of Ne and Ar if you first calculate the internal energy for He?

9.3 Entropy of an ideal gas

Calculate the molar entropy of Ar at 200 K, 300 K and 500K in a volume $V = 1000$ cm^3. Treat Ar as an ideal gas. What is the difference if you exchange Ar by Kr?

9.4 Vibrational partition function of $^{35}Cl_2$

The standard frequency of a $^{35}Cl_2$ molecule is $1.663 \cdot 10^{13}$ s^{-1}.

(a) Calculate θ_ν.

(b) Calculate $\exp(-\epsilon_{vib}(\nu)/kT) = \exp(-\nu\theta_\nu/T)$ for $\nu = 1, 2, 3$ at 300 K.

(c) Sketch the dependency of the number of molecules in a specific vibrational state with respect to ν.

9.5 Rotational partition function of $^{35}Cl_2$

Calculate the characteristic rotational temperature θ_{rot} of a $^{35}Cl_2$ molecule with a Cl-Cl distance of 0.199 nm. What is the value of the rotational partition function at 300 K.

9.6 Partition function of HCN

Spectroscopic measurements of the HCN vibration yielded the following wave numbers: $\tilde{\nu_1} = 2096{,}70$ cm^{-1}, $\tilde{\nu_2} = 713{,}46$ cm^{-1} (two-fold degenerated), $\tilde{\nu_3} = 3311{,}47$ cm^{-1}. The moment of inertia is $1.8816 \cdot 10^{-46}$ kg m^2.

(a) Calculate c_V at 293 K, 500 K and 1000 K.

(b) Calculate the entropy S at 1 bar and 1000 K.

(*Hint: treat C as ^{12}C and N as ^{14}N.*)

9.7 Influence of the symmetry on the partition function

CO_2 is a linear molecule, SO_2 an angulated molecule. Which molecules has the highest partition function product $z_{vib} \cdot z_{rot}$ at room temperature?