Project 1: A gas of sodium atoms at high temperature

In this project, we consider different states of the element sodium (Na) in the gas phase at high temperatures. The sodium atoms are in the ground state and the ionization energy for the process $Na \rightarrow Na^{+} + e^{-}$ is $D_i = 5{,}14\ eV$. The electron spin creates the degeneracy $g_e = 2$ for the electron $g_{e,Na} = 2$ for Na, whereas $g_{e,Na^{+}} = 1$ for the ionized atom. The disassociationenergy for the cleavage of the dimer $Na_2 \rightarrow 2Na$ is $D_e = 0{,}75\ eV$ and includes the zeropoint contribution from the vibration of the dimer. The characteristic rotational- and vibrationaltemperatures for Na_2 is $\theta_{vib} = 229\ K$ and $\theta_{rot} = 0{,}221\ K$. Due to the spin of the electron, we have that $g_{e,Na2} = 1$ for Na_2. We ignore the effects of nuclear spin.

1: Specify expressions for the canonical partition functions for respectively a single sodium atom and N non-interacting sodium atoms in the gaseous phase, neglecting electronic degrees of freedom and spin.

2: Calculate expressions for the Helmholtz energy F, the internal energy U and the entropy S of N ideal Na-atoms in the gaseous phase.

In a gas of sodium steam, Na2 appears as dimers, which are cleaved accordingly:

$$Na_2 \rightleftharpoons$$

The dimer Na_2 possesses translational- vibrational- and rotational degrees of freedom. The rotational degrees of freedom are treated classicaly by the formula for the energy $E_{rot} = \frac{I}{2}\omega^2$, where I is the moment of inertia and ω is its rotational frequency.

3: Explain why the rotational partition function for a molecule can be written as

$$z_{rot} = \frac{T}{2\theta_{rot}}$$

and name an expression for the rotationaltemperature θ_{rot}.

4: Write down an expression for the canonical partition function for N ideal Na2 gas molecules, when the rotational contribution is treated classically, and all inner degrees of freedom are treated quantum mechanically. Use this and earlier results to calculate an expression for the equilibrium constant K_d for the reaction (1) and calculate its value at $T = 1000K$.