Illustration

Exercise 2.1-2

Do the Math for the Formation Entropy

Do the Math needed for going from the first to the second formula:

- **First formula:**

$$F = -kT \cdot \ln Z = kT \cdot \sum_i \left(\frac{h\omega_i}{4\pi \cdot kT} + \ln\left(1 - \exp - \frac{h\omega_i}{2\pi \cdot kT}\right)\right)$$

- **Second formula:**

$$S = k \cdot \sum_i \left(-\ln\left(1 - \exp \frac{h\omega_i}{2\pi \cdot kT}\right) + \frac{\frac{h\omega_i}{2\pi \cdot kT}}{\exp\left(\frac{h\omega_i}{2\pi \cdot kT} - 1\right)}\right)$$

Now, using the approximations referred to, derive the **Final formula**

$$S_F = k \cdot \sum_i \ln \frac{\omega_i}{\omega'_i}$$

Discuss the quality of the approximations

- (Hint: Use some real numbers or order of magnitudes for e.g. Debye temperatures, vacancy concentrations etc.)

Link to the Solution