

[tex88] Classical rotational entropies of HCl and N₂ gases

Under the assumption (to be justified quantum mechanically) that only the rotational modes perpendicular to the axis of a two-atomic molecule are activated, its classical rotational motion is described by a Hamiltonian with two degrees of freedom,

$$H_R = \frac{p_\theta^2}{2I_1} + \frac{p_\phi^2}{2I_1 \sin^2 \theta},$$

where $0 \leq \theta \leq \pi$, $-\infty < p_\theta, p_\phi < +\infty$. The range of the other angle is $0 \leq \phi \leq 2\pi$ for heteronuclear molecules (e.g. HCl) and $0 \leq \phi \leq \pi$ for homonuclear molecules (e.g. N₂).

(a) Calculate the canonical partition function Z_R^N for the rotational motion of a gas of N HCl molecules and a gas of N N₂ molecules.

(b) Calculate the difference in rotational entropy and in rotational internal energy of the two gases when both are at the same temperature.

Note the different roles of θ here and in [tex84]. There $\phi, \cos\theta$ and here θ, p_θ are a pair of canonically conjugate coordinates.

Solution: