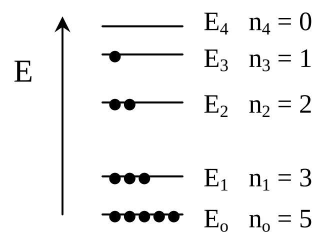
Entropy and the Partition Function (from $S = -k\Sigma\, p_i \ln p_i$)

$$S = \frac{k}{\mathcal{N}} \ln \mathcal{W}_{max}$$ (Canonical ensemble)



$$\mathcal{W} = \frac{\mathcal{M}!}{n_o!n_1!n_2!\ldots}$$

$$S = -k \sum_{i=0}^{\infty} p_i \ln p_i$$ (sum over all energy states)

$$p_i = \frac{e^{-E_i/kT}}{Q} \qquad \ln p_i = -\ln Q - {}^{E_i}/_{kT}$$

$$S = -k \sum_{i=0}^{\infty} p_i \ln p_i = k\, \Sigma\, p_i \ln Q + \frac{\Sigma p_i E_i}{T}$$

$$S = k \ln Q + \frac{\langle E \rangle}{T}$$

$$S = k \ln Q + \frac{U - U(0)}{T}$$ U(0) at 0 K

---

ideal gas: $U - U(0) = {}^3/_2\, nRT = {}^3/_2\, NkT \qquad S = k \ln Q + {}^3/_2\, nR$

$$Q = \frac{q^N}{N!} \qquad N! \cong ({}^N/e)^N \qquad Q \cong \left(\frac{qe}{N}\right)^N$$ ideal monatomic: $q_t = \frac{(2\pi mkT)^{3/2}}{h^3} V$

$$S = Nk \ln\left(\frac{qe}{N}\right) + {}^3/_2\, nR = nR \ln\left[\frac{(2\pi mkT)^{3/2} e}{Nh^3} V\right] + {}^3/_2\, nR$$ $m \sim$ kg molecule^{-1}, $V \sim m^3$

---

per mole: $N = N_A$ $\quad n = 1$ mol $\quad N_A k = R$ $\quad {}^3/_2 = \ln e^{3/2}$

$$S_m = R \ln\left[\frac{(2\pi mkT)^{3/2} e^{5/2}}{N_A h^3} V_m\right]$$ Sackur-Tetrode Equation

---

$$S_m = R \ln V_m + {}^3/_2\, R \ln T + {}^3/_2\, R \ln \mathcal{M} + R \ln\left[\frac{(2\pi k(1\text{ kg}/1000\text{ g})/N_A)^{3/2} e^{5/2} (1\text{ m}^3/1000\text{ L})}{N_A h^3}\right]$$

$$S_m = R \ln(V_{m/L}) + {}^3/_2\, R \ln T + {}^3/_2\, R \ln(\mathcal{M}_{/g\ mol^{-1}}) + 11.1037 \text{ J K}^{-1} \text{ mol}^{-1}$$

---

cst. T: $\Delta S_m = R \ln({}^{V_2}/_{V_1})$ cst. V: $\Delta S_m = {}^3/_2\, R \ln({}^{T_2}/_{T_1}) = C_v \ln({}^{T_2}/_{T_1})$

$P^\circ = 1$ bar $\qquad V_m^\circ = RT/P^\circ = 0.0247890\ m^3 = 24.7890$ L at 298.15 K

$S^\circ_{m,298.15\,K} = 26.6929 + 71.0587 + {}^3/_2\, R \ln(\mathcal{M}_{/g\ mol^{-1}}) + 11.1037 \text{ J K}^{-1} \text{ mol}^{-1}$

(translation)