

THERMODYNAMIC IDENTITIES

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$$C_V = \left(\frac{\partial U}{\partial T} \right)_V ; \quad C_P = \left(\frac{\partial H}{\partial T} \right)_P ; \quad C_P = C_V + TV\alpha\gamma_V$$

Specific heat

$$\gamma \equiv V \left(\frac{\partial P}{\partial U} \right)_V = \frac{V}{C_V} \left(\frac{\partial P}{\partial T} \right)_V = - \left(\frac{\partial \ln T}{\partial \ln V} \right)_S$$

Grüneisen parameter

$$\left(\frac{\partial T}{\partial V} \right)_S = -T \left(\frac{\partial P}{\partial T} \right)_V / \left(\frac{\partial U}{\partial T} \right)_V$$

Isochores $\rightarrow$ Isentropes

$$\left(\frac{\partial T}{\partial P} \right)_S = \frac{TV\alpha}{C_P} = \frac{T\gamma}{K_S}$$

Adiabatic temperature profile

$$\alpha \equiv \frac{1}{V} \left(\frac{\partial V}{\partial T} \right)_P = \gamma \rho C_P / K_T$$

Thermal expansion coefficient

$$K_T \equiv B \equiv -V \left(\frac{\partial P}{\partial V} \right)_T = \rho \left(\frac{\partial P}{\partial \rho} \right)_T$$

Bulk modulus

$$K_S \equiv -V \left(\frac{\partial P}{\partial V} \right)_S = (1 + \alpha\gamma T) K_T$$

Adiabatic bulk modulus

$$\gamma_V \equiv \left(\frac{\partial P}{\partial T} \right)_V = \alpha K_T$$

Thermal pressure coefficient

$$P(V, T) - P(V, T_0) = \int_{T_0}^T \alpha(V, T') K_T(V, T') dT'$$

Thermal pressure

$$P(V, T) = - \left(\frac{\partial U}{\partial V} \right)_T + T \left(\frac{\partial P}{\partial T} \right)_V$$

Total pressure

$$\left(\frac{\partial V}{\partial T} \right)_P = - \left[\left(\frac{\partial U}{\partial P} \right)_T + P \left(\frac{\partial V}{\partial P} \right)_T \right] \frac{1}{T} = \alpha V = \frac{\gamma_V}{K_T} V$$

Combined relations

$$U = - \left(\frac{\partial(\beta F)}{\partial \beta} \right)_V$$

$$dU = T dS - P dV$$

$$F = U - TS$$

$$dF = -S dT - P dV$$

$$G = U - TS + PV$$

$$dG = -S dT + V dP$$

$$H = U + PV = -T^2 \left(\frac{\partial(G/T)}{\partial T} \right)_P \rightarrow \Delta \left(\frac{G}{T} \right)_{P_0} = - \int_{T_0}^{T_1} \frac{H(P_0, T)}{T^2} dT$$

Gibbs-Helmholtz
(thermodynamic integration)

$$\beta_2 F_2 - \beta_1 F_1 = \int_{\beta_1}^{\beta_2} U(\beta) d\beta$$

Helmholtz Free Energy difference
(thermodynamic integration)

$$\langle K \rangle = -\frac{1}{2} \left\langle \sum_{j=1}^N \mathbf{r}_j \cdot \mathbf{F}_j^{\text{tot}} \right\rangle = \frac{3}{2} N k_B T$$

Virial theorem

$$P = - \left(\frac{\partial F}{\partial V} \right)_T = - \left(\frac{\partial U}{\partial V} \right)_S = \frac{N k_B T}{V} + \frac{1}{3V} \left\langle \sum_{i=1}^N \mathbf{r}_i \cdot \mathbf{f}_i \right\rangle$$

Pressure

MAXWELL RELATIONS

$$\left(\frac{\partial T}{\partial V}\right)_S = -\left(\frac{\partial P}{\partial S}\right)_V$$

$$\left(\frac{\partial T}{\partial P}\right)_S = \left(\frac{\partial V}{\partial S}\right)_P$$

$$\left(\frac{\partial S}{\partial V}\right)_T = \left(\frac{\partial P}{\partial T}\right)_V$$

$$\left(\frac{\partial S}{\partial P}\right)_T = -\left(\frac{\partial V}{\partial T}\right)_P$$

OTHER RELATIONS

$$\left(\frac{\partial U}{\partial T}\right)_P = C_P - PV\alpha$$

$$\left(\frac{\partial U}{\partial P}\right)_T = \frac{C_V - C_P}{\alpha K_T} + \frac{PV}{K_T}$$

$$\left(\frac{\partial U}{\partial P}\right)_V = \frac{C_V}{\alpha K_T}$$

$$\left(\frac{\partial U}{\partial V}\right)_P = \frac{C_P}{V\alpha} - P$$

$$\left(\frac{\partial U}{\partial V}\right)_T = \frac{C_P - C_V}{V\alpha} - P$$