

Table E.1 Thermodynamic notation and definitions (note that parameters V , S , U , H , F and G refer to arbitrary mass, m , but C_V and C_P refer to unit mass)

Specific heat, constant P	$C_P = (T/m)(\partial S/\partial T)_P$
constant V	$C_V = (T/m)(\partial S/\partial T)_V$
	$C'_S = (\partial \ln C_V/\partial \ln V)_S$; $C'_T = (\partial \ln C_V/\partial \ln V)_T$
Helmholtz free energy	$F = U - TS$
Gibbs free energy	$G = U - TS + PV$
Enthalpy	$H = U + PV$
Bulk modulus, adiabatic	$K_S = -V(\partial P/\partial V)_S$
	$K'_S = (\partial K_S/\partial P)_S$; $K''_S = (\partial K'_S/\partial P)_S$
isothermal	$K_T = -V(\partial P/\partial V)_T$
	$K'_T = (\partial K_T/\partial P)_T$; $K''_T = (\partial K'_T/\partial P)_T$
Pressure	P
	$q = (\partial \ln \gamma/\partial \ln V)_T = (\partial \ln(\gamma C_V)/\partial \ln V)_S$
	$q_S = (\partial \ln \gamma/\partial \ln V)_S = q - C'_S$
Heat	Q
Entropy	$S = \int dQ/T$
Temperature	T
Internal energy	U
Volume	V
Volume expansion coefficient	$\alpha = (1/V)(\partial V/\partial T)_P$
Grüneisen parameter	$\gamma = \alpha K_T/\rho C_V = \alpha K_S/\rho C_P$
Anderson-Grüneisen parameter, adiabatic	$\delta_S = -(1/\alpha)(\partial \ln K_S/\partial T)_P = (\partial \ln(\alpha T/C_P)/\partial \ln V)_S$
isothermal	$\delta_T = -(1/\alpha)(\partial \ln K_T/\partial T)_P = (\partial \ln \alpha/\partial \ln V)_T$
Density	$\rho = m/V$
	$\lambda = (\partial \ln q/\partial \ln V)_T$

Table E.2 First order derivatives of thermodynamic parameters

Differential element	Constant									
	T	P	V	S	U	H	F	G		
∂T	-	1	1	γT	$P - \alpha K_T T$	$1 - \alpha T$	P	1		
∂P	$-K_T/V$	-	$\alpha K_T = \gamma \rho C_V$	K_S	$-\rho C_V(K_S - \gamma P)$	$-\rho C_P$	$K_T(S/V + \alpha P)$	S/V		
∂V	1	αV	-	-V	m_{C_V}	$\alpha V(1 + 1/\gamma)$	-S	$\alpha V - S/K_T$		
∂S	$\alpha K_T = \gamma \rho C_V$	$m_{C_P/T}$	$m_{C_V/T}$	-	$m_{C_V} P/T$	$m_{C_P/T}$	$m_{C_V}(P/T - \gamma S/V)$	$m_{C_P/T} - \alpha S$		
∂U	$\alpha K_T T - P$	$m_{C_P} - \alpha VP$	m_{C_V}	PV	-	$m_{C_P} - PV\alpha$	$m_{C_V} P - S\alpha K_T T$	$m_{C_P} - \alpha TS - P\alpha V$		
∂H	$-K_T(1 - \alpha T)$	m_{C_P}	$m_{C_V}(1 + \gamma)$	$K_S V$	$m_{C_V}[P(1 + \gamma) - K_S]$	-	$S K_T(1 - \alpha T) + m_{C_V} P(1 + \gamma)$	$m_{C_P} + S(1 - \alpha T)$		
∂F	-P	$-S - \alpha VP$	-S	$PV - \gamma TS$	$\rho C_V(\gamma TS - PV) - PS$	$-S(1 - \alpha T)$	-	$-S(1 - P/K_T) - P\alpha V$		
∂G	$-K_T$	-S	$-S + \alpha K_T V$	$K_S V - \gamma TS$	$m_{C_V}(\gamma TS V + \gamma P - K_S) - PS$	$-S(1 - \alpha T) - m_{C_P}$	$S(K_T - P) + PV\alpha K_T$	-		

Table E.3 Thermodynamic derivatives extended to second order at constant T, P, V and S

Differential element	Constant			
	T	P	V	S
∂T	-	1	1	γT
∂P	$-K_T/V$	-	$\alpha K_T = \gamma \rho C_V$	K_S
∂V	1	αV	-	$-V$
∂S	$\alpha K_T = \gamma \rho C_V$	$m C_P/T$	$m C_V/T$	-
∂U	$\alpha K_T - P$	$m C_P - \alpha VP$	$m C_V$	PV
∂H	$-K_T(1 - \alpha T)$	$m C_P$	$m C_V(1 + \gamma)$	$K_S V$
∂F	-P	$-S - \alpha VP$	-S	PV - γTS
∂G	$-K_T$	-S	$-S + \alpha K_T V$	$K_S V - \gamma TS$
$\partial \alpha$	$\alpha \delta_T V = -(\partial K_T / \partial T)_P / K_T V$	$\alpha^2(2\delta_T - K_T + C_T / \gamma \alpha T)$	$\alpha^2(\delta_T - K_T + C_T / \gamma \alpha T)$	$-\alpha[K_S - 1 + q + \gamma \alpha T(\delta_S + q)]$
∂K_T	$-K_T K_T V$	$-\alpha K_T \delta_T = K_T^2 (\partial \alpha / \partial P)_T$	$\alpha K_T(K_T - \delta_T)$	$K_T [K_T + \gamma \alpha T(K_T - \delta_T)]$
∂K_S	$(-K_T V)(K_S + \gamma \alpha T \delta_S)$	$-\alpha K_S \delta_S$	$\alpha K_T(K_S - \delta_S)$	$K_S K_S$
∂C_V	$(C_V/M)C_T = (C_V/M)(1 - q + \delta_T - K_T)$	$(C_P C_T - C_V C_S) / \gamma T$	$(C_V / \gamma T)(C_T - C_S)$	$-T C_V (\partial \gamma / \partial T)_V$
∂C_P	$(C_P/M)[C_T + \gamma \alpha T(q + \delta_T)] / (1 + \gamma \alpha T)$	$(C_P / \gamma T)[C_T - C_S + \gamma \alpha T \times (\delta_T - \delta_S + C_T)]$	$(C_P / \gamma T)[C_T(1 + \gamma \alpha T) + [\gamma^2 \alpha T + (\gamma \alpha T)^2 \times (q - 1) - C_S^2] / (1 + \gamma \alpha T)]$	$-C_P T (\partial \gamma / \partial T)_V + \gamma \alpha T(\delta_S + q)$
$\partial \gamma$	$\gamma q / V$	$\gamma \alpha q + C_S^2 / T$	C_S^2 / T	$-\gamma(q - C_S)$

Table E.4 Relationships between derivatives

$$K_S/K_T = C_P/C_V = 1 + \gamma\alpha T \quad (\text{E.1})$$

$$K'_T = K'_S(1 + \gamma\alpha T) + \gamma\alpha T[3q - 2 - \gamma + \gamma(\partial \ln C_V/\partial \ln T)_V] \quad (\text{E.2})$$

$$K'_S = K'_T(1 + \gamma\alpha T) - \gamma\alpha T(\delta_S + \delta_T + q) \quad (\text{E.3})$$

$$\delta_S = -(1/\alpha)(\partial \ln K_S/\partial T)_P = K'_S - 1 + q - \gamma - C'_S = (\partial \ln(\alpha T/C_P)/\partial \ln V)_S \quad (\text{E.4})$$

$$\begin{aligned} \delta_T &= -(1/\alpha)(\partial \ln K_T/\partial T)_P = K'_T - 1 + q + C'_T = (\partial \ln \alpha/\partial \ln V)_T \\ &= (\delta_S + C'_T)(1 + \gamma\alpha T) + \gamma + C'_S + \gamma\alpha T(2q - 1) \end{aligned} \quad (\text{E.5})$$

$$C'_S = C'_T - \gamma(\partial \ln C_V/\partial \ln T)_V = (\partial \gamma/\partial \ln T)_V \quad (\text{E.6})$$

$$C'_T = \gamma(\partial \ln(\gamma C_V)/\partial \ln T)_V \quad (\text{E.7})$$

$$q_S = q - C'_S \quad (\text{E.8})$$

$$(\partial \ln(\alpha K_T)/\partial \ln V)_T = \delta_T - K'_T = -(1/\alpha)(\partial \ln K_T/\partial T)_V \quad (\text{E.9})$$

$$(\partial \ln(\alpha K_T)/\partial \ln T)_V = (\partial \ln(\gamma C_V)/\partial \ln T)_V = C'_T/\gamma \quad (\text{E.10})$$

$$(\partial(\alpha K_T)/\partial T)_P = K_T(\partial \alpha/\partial T)_V \quad (\text{E.11})$$

$$(\partial \ln(\alpha K_T)/\partial \ln V)_S = q - 1 \quad (\text{E.12})$$

$$(\partial \ln(\alpha K_S)/\partial \ln V)_S = q - 1 + \gamma\alpha T(\delta_S + q) \quad (\text{E.13})$$

$$(\partial \ln(\gamma\alpha T)/\partial \ln V)_T = \delta_T + q \quad (\text{E.14})$$

$$(\partial \ln(\gamma\alpha T)/\partial \ln V)_S = (1 + \gamma\alpha T)(\delta_S + q) \quad (\text{E.15})$$

$$(\partial K'_T/\partial T)_P = \alpha\delta_T[\delta_T - K'_T + (\partial \ln \delta_T/\partial \ln V)_T] \quad (\text{E.16})$$

$$(\partial K'_S/\partial T)_P = \alpha\delta_S[\delta_S - K'_S + (\partial \ln \delta_S/\partial \ln V)_S] \quad (\text{E.17})$$

$$(\partial \delta_T/\partial \ln V)_T = -K_T K''_T + \lambda q + (\partial C'_T/\partial \ln V)_T \quad (\text{E.18})$$

$$(\partial \delta_S/\partial \ln V)_S = -K_S K''_S - \gamma q_S + (\partial q_S/\partial \ln V)_S \quad (\text{E.19})$$

$$(\partial C_P/\partial P)_T = -(\partial(\alpha/\rho)/\partial \ln T)_P \quad (\text{E.20})$$