

P XXX/00 Abbreviations used in Biothermodynamics

a, b, c, d, e, f, g, x, y, z,	stoichiometric coefficients
act	actual conditions, e.g. T_{act}
a_j	ion size parameter in $[10^{-8} \text{ cm}]$
(am)	amorphous state
(aq)	aqueous state
[atm]	standard atmosphere: $1 [\text{atm}] \hat{=} 101325[\text{Pa}] \hat{=} 760[\text{Torr}] \hat{=} 1.01325[\text{bar}]$
a_w	water activity
bar	$1 [\text{bar}] \hat{=} 10^5[\text{Pa}] \hat{=} 0.986923[\text{atm}] \hat{=} 750.062 [\text{Torr}]$
c	denotes combustion
c_0	speed of light in vacuum = $299792458 \text{ ms}^{-1}$
c_i	concentration of chemical species i
c_i^0	standard concentration of species j [1 mol/dm^3]
e^-	electron
e	base of natural logarithm = 2.71828182846
e	elementary charge = $1.60217733(49) \cdot 10^{-19} \text{ Coulomb}$
emf	electromotive force
eq	equilibrium
exp	exponential function to base e
f	denotes thermochemical quantity associated with the formation of a substance from elements in their reference state, e.g. Gf, Hf, Sf
f_j	Debye-Hückel activity correction factor
(g)	gaseous state
g_n	standard acceleration = 9.80665 ms^{-2}
h	Planck constant = $6.6260755(40) \cdot 10^{-34} \text{ Js}$
h	surplus charge of biomolecule
i, j	chemical species designation
k	Boltzmann constant = $1.380658(12) \cdot 10^{-23} \text{ JK}^{-1}$
(l)	liquid state
[l]	liter
ln	natural logarithm = $2.30258509299 \cdot {}_{10}\log$
ln 10	natural logarithm of 10 = 2.30258509299
m	slope of linear function
n	number of electrons transferred
neq	non-equilibrium
ox	oxidized
p	pressure
p^0	standard state pressure 1[atm] (earlier), 1[bar] (today)
pe	$-\log \{e^-\}$; electron activity
pe^0	electron activity reference state = $\frac{1}{n} \cdot \log K_{\text{eq}} \hat{=} \frac{F \cdot E^0}{2.3026 R \cdot T}$
pH	$-\log \{H^+\}$, negative logarithm of proton activity
pK	$-\log K$
$\pm q$	number of protons transferred, + if they are produced, - if they are consumed

r	denotes thermodynamic quantity associated with a reaction, e.g. $\Delta G_r, \Delta H_r, \Delta S_r$
ref	reference state e.g. $T_{ref} = 298.15[K]$
red	reduced
(s)	solid state
$v_{i,j}$	stoichiometric coefficients of species i, j
x, y, z	stoichiometric coefficients
y_1	intercept on y-axes
z_j	charge of species j
[]	designates concentration, or monomer unit
{ }	designates activity
< >	designates hypothetical unit molecule, e.g. for biomass
$[-C_aH_b-]$	designates repetitive molecular fragment, e.g. monomer molecule
$[C(H)_2(C)(CO)]$	designates group increment
$\alpha_0, \alpha_1, \alpha_2$	acid-base pair distribution coefficients
$\gamma_0, \gamma_1, \gamma_2, \epsilon_0, \epsilon_1, \vartheta_0, \vartheta_1, \vartheta_2$	for mono- and diprotic acids
Σ	sum of terms
Π	product of terms
ϵ_T	temperature-dependent dielectric coefficient of water
π	ratio of circumference to diameter of a circle = 3.14159265359
$\sigma = 2\pi^5 k^4 / 15h^3 c^2$	Stefan-Boltzmann constant = $5.67051(19) \cdot 10^{-8} \text{ Wm}^{-2} \text{ K}^{-4}$
σ	symmetry factor
II, II-, V+, U, R, etc.	designates oxidation states
+, -, 2-, 3+, h, etc.	designates ionic charges
$^{\circ}$	denotes standard state conditions with reactants in their pure state at a pressure of 1 [atm] if the reactants are gases or 1-molal concentration if the reactants are solutes
$^{\circ}$	denotes standard state except for 1 reactant (e.g. pH \neq 0)
A, B, C, D, ...X, Y, Z	chemical species
A, B	Debye-Hückel-Onsager parameters $A=1.82 \cdot 10^6 (\epsilon_T \cdot T)^{-3/2}$, $B=50.3 \cdot (\epsilon_T \cdot T)^{-1/2}$
A^-, A^{2-}	anions of mono- and diprotic acids
[°C]	temperature in degree Celcius = $T/K - 273.15$
C_r	sum of inorganic carbonate species $= [CO_{2(aq)}] + [H_2CO_{3(aq)}] + [HCO_{3(aq)}^-] + [CO_{3(aq)}^{2-}]$
C, H, O, N, P, S	most common chemical elements in organic biomolecules
[Da]	Dalton
E	electrochemical potential in [V]=emf
E°	standard emf= electrochemical reference potential $[V] = -\Delta G_r^{\circ} / n \cdot F \hat{=} 2.3026 \cdot R \cdot T \cdot p_{\epsilon}^{\circ} / F$
E°	standard emf at pH \neq 0
F	Faraday's constant = $96.485309 \text{ [kJ} \cdot \text{mol}^{-1} \cdot \text{V}^{-1}]$
Gf°	standard free energy of formation [kJ/mol]
ΔGf°	standard Gibbs free energy change of formation
ΔG_r°	change of Gibbs free energy of reaction at standard conditions $= -R \cdot T \cdot \ln K^{\circ}$

$\Delta G_r^{0'}$	change of Gibbs free energy of reaction at standard conditions except for one reactant (e.g. at $\text{pH} \neq 0$)
ΔG_r	change of Gibbs free energy of reaction at actual conditions
H^+	proton
Hf^0	standard enthalpy of formation [kJ/mol]
ΔHf^0	standard enthalpy change of formation
ΔH_r^0	change of enthalpy of reaction at standard conditions
ΔH_r	change of enthalpy of reaction at actual condition
HA, H_2A	mono- and diprotic acids, protonated
I	ionic strength = $\frac{1}{2} \sum_j c_j \cdot z_j^2$ [mol/l]
IAP	ionic activity product
[J]	Joule
[K]	temperature in Kelvin degree
K	dissociation, equilibrium or solubility coefficient
K'_1, K'_2	temperature and/or ionic strength corrected dissociation coefficient
K_a^0	thermodynamic acid dissociation coefficient
K_D	Ostwald coefficient = $K_H \cdot R \cdot T$ [-]
$K_{\text{eq}} \hat{=} K^0$	thermodynamic equilibrium coefficient
$\log K_{\text{eq}}$	= $-\Delta G_r^0 / 2.3026 \cdot R \cdot T$
K_{Hb}	Henry's law constant [$\text{mol} \cdot \text{l}^{-1} \cdot \text{atm}^{-1}$]
K'_s	thermodynamic solubility product for standard conditions
K_s	actual solubility product for $I \neq 1$
K_s^0	operational solubility product for standard conditions at $I=1$
K_w	dissociation coefficient of water
[kJ]	kilojoule = 10^3 Joule
L_T	sum of inorganic sulfate species = $[\text{H}_2\text{SO}_4] + [\text{HSO}_4^-] + [\text{SO}_4^{2-}]$
M	sum of minor elements in organic molecule
P	reaction-product
[Pa]	1 Pascal $\hat{=} 9.86923 \cdot 10^{-6}$ [atm] $\hat{=} 7.50062 \cdot 10^{-3}$ [Torr]
Q	ratio of actual activity products of reactants
Q'	ratio of actual activity products of reactants excluding protons (or/and electrons in half-reactions)
-R-	rest of organic molecule, mostly C-entity
R^+	average of oxidation state of M
R	gas constant = $8.31451 \cdot 10^{-3}$ [kJ·mol ⁻¹ ·K ⁻¹] (concentration basis) = $82.057844 \cdot 10^{-3}$ [atm·l·mol ⁻¹ ·K ⁻¹] (pressure basis)
S	substrate
S_f^0	standard entropy of formation [J/K·mol]
ΔS_f^0	standard entropy change of formation
ΔS_r^0	change of entropy of reaction at standard conditions
ΔS_r	change of entropy of reaction at actual conditions
S_T	sum of inorganic sulfide species = $[\text{H}_2\text{S}] + [\text{HS}^-] + [\text{S}^{2-}]$
T	thermodynamic temperature in [K]

U	oxidation state (number of) carbon in an organic molecule
[V]	volt
V_0	molar volume of ideal gas (at $p^0=1$ bar, $T=273.15$ K) =22.71108 [l·mol ⁻¹], $\hat{=} 22.41409$ [l·mol ⁻¹] for $p^0=1$ [atm] and $T=273.15$ K; for $p^0=1$ [atm] and $T=298.15$ K, $V_0=24.46554$ [l·mol ⁻¹]
W	number of possible structural configurations
X, Y	chemical species