

**P XXX/00 Abbreviations used in Biothermodynamics**

a, b, c, d, e, f, g, x, y, z,	stoichiometric coefficients
act	actual conditions, e.g. $T_{\text{act}}$
$a_j$	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 [ $1 \text{ mol/dm}^3$ ]
$e^-$	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 = $9.80665 \text{ ms}^{-2}$
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 = $\frac{1}{n} \cdot \log \text{Keq} \hat{=} \frac{F \cdot E^0}{2.3026 R \cdot T}$
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. $T_{\text{ref}} = 298.15 [\text{K}]$
red	reduced
(s)	solid state

$v_{ij}$	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
$\Sigma$	sum of terms
$\Pi$	product of terms
$\epsilon_T$	temperature-dependent dielectric coefficient of water
$\pi$	ratio of circumference to diameter of a circle = 3.14159265359
$\sigma = 2\pi^5 k^4 / 15h^3 c^2$	Stefan-Boltzmann constant = $5.67051(19) \cdot 10^{-8} \text{ Wm}^{-2} \text{ K}^{-4}$
$\sigma$	symmetry factor
II, II-, V+, U, R, etc.	designates oxidation states
+, -, 2-, 3+, h, etc.	designates ionic charges
$^0$	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
$E^0$	standard emf= electrochemical reference potential
	$[V] = -\Delta G_r^0 / n \cdot F \hat{=} 2.3026 \cdot R \cdot T \cdot p_e^0 / F$
$E^{\circ}$	standard emf at pH $\neq$ 0
F	Faraday's constant = $96.485309 \text{ [kJ} \cdot \text{mol}^{-1} \cdot \text{V}^{-1}]$
$Gf^0$	standard free energy of formation [kJ/mol]
$\Delta Gf^0$	standard Gibbs free energy change of formation
$\Delta G_r^0$	change of Gibbs free energy of reaction at standard conditions
	$= -R \cdot T \cdot \ln K^0$
$\Delta G_r^{\circ}$	change of Gibbs free energy of reaction at standard conditions except for one reactant (e.g. at pH $\neq$ 0)
$\Delta G_r$	change of Gibbs free energy of reaction at actual conditions
$H^+$	proton
$Hf^0$	standard enthalpy of formation [kJ/mol]
$\Delta Hf^0$	standard enthalpy change of formation

$\Delta H_r^0$	change of enthalpy of reaction at standard conditions
$\Delta H_r$	change of enthalpy of reaction at actual condition
HA, H <sub>2</sub> A	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 <sub>1</sub> <sup>'</sup> , K <sub>2</sub> <sup>'</sup>	temperature and/or ionic strength corrected dissociation coefficient
K <sub>a</sub> <sup>0</sup>	thermodynamic acid dissociation coefficient
K <sub>D</sub>	Ostwald coefficient = K <sub>H</sub> · R · T [-]
K <sub>eq</sub> ≙ K <sup>0</sup>	thermodynamic equilibrium coefficient
log K <sub>eq</sub>	= -ΔG <sub>r</sub> <sup>0</sup> / 2.3026 · R · T
K <sub>Hb</sub>	Henry's law constant [mol · l <sup>-1</sup> · atm <sup>-1</sup> ]
K <sub>S</sub>	thermodynamic solubility product for standard conditions
K <sub>S</sub> <sup>'</sup>	actual solubility product for I ≠ 1
K <sub>S</sub> <sup>0</sup>	operational solubility product for standard conditions at I=1
K <sub>w</sub>	dissociation coefficient of water
[kJ]	kilojoule = 10 <sup>3</sup> Joule
L <sub>T</sub>	sum of inorganic sulfate species = [H <sub>2</sub> SO <sub>4</sub> ] + [HSO <sub>4</sub> <sup>-</sup> ] + [SO <sub>4</sub> <sup>2-</sup> ]
M	sum of minor elements in organic molecule
P	reaction-product
[Pa]	1 Pascal ≙ 9.86923 · 10 <sup>-6</sup> [atm] ≙ 7.50062 · 10 <sup>-3</sup> [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 <sup>+</sup>	average of oxidation state of M
R	gas constant = 8.31451 · 10 <sup>-3</sup> [kJ · mol <sup>-1</sup> · K <sup>-1</sup> ] (concentration basis) = 82.057844 · 10 <sup>-3</sup> [atm · l · mol <sup>-1</sup> · K <sup>-1</sup> ] (pressure basis)
S	substrate
Sf <sup>0</sup>	standard entropy of formation [J/K · mol]
ΔSf <sup>0</sup>	standard entropy change of formation
ΔS <sub>r</sub> <sup>0</sup>	change of entropy of reaction at standard conditions
ΔS <sub>r</sub>	change of entropy of reaction at actual conditions
S <sub>T</sub>	sum of inorganic sulfide species = [H <sub>2</sub> S] + [HS <sup>-</sup> ] + [S <sup>2-</sup> ]
T	thermodynamic temperature in [K]
U	oxidation state (number of) carbon in an organic molecule
[V]	volt
V <sub>0</sub>	molar volume of ideal gas (at p <sup>0</sup> =1 bar, T=273.15 K) = 22.71108 [l · mol <sup>-1</sup> ], ≙ 22.41409 [l · mol <sup>-1</sup> ] for p <sup>0</sup> =1 [atm] and T=273.15 K; for p <sup>0</sup> =1 [atm] and T=298.15 K, V <sub>0</sub> =24.46554 [l · mol <sup>-1</sup> ]
W	number of possible structural configurations
X, Y	chemical species