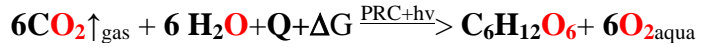


Calculate ΔH_r , ΔS_r , ΔG_r at standard conditions 298.15 K. Reaction is **exothermic**, **athermic**, **endothermic**? CO_2 gas assimilation reaction in green plants with blue and red photons $E=h\nu$ absorption in photosynthetic reaction center $\text{PRC}+h\nu$ for production $6\text{O}_{2\text{aqua}}$ and $\text{C}_6\text{H}_{12}\text{O}_6$ using the data table! Mention whether the reaction will be **exoergic** or **endoergic**!

Initial compounds => products glucose + oxygen

Substance	ΔH_r° , kJ/mol	ΔS_r° , J/mol/K
$\text{C}_6\text{H}_{12}\text{O}_6(\text{aq})$	-1263.78	269.45
$\text{O}_{2\text{aqua}}$	-11.715	110.876
H_2O	-285.85	69.9565
$\text{CO}_2\uparrow_{\text{gas}}$	-393.509	213.74



<= biooxidation (Krebs cycle, Glycolyse)

$$1. \Delta H_{\text{reaction}} = \sum \Delta H^\circ_{\text{products}} - \sum \Delta H^\circ_{\text{initial compounds}}$$

$$2. \Delta S_{\text{reaction}} = \sum \Delta S^\circ_{\text{products}} - \sum \Delta S^\circ_{\text{initial compounds}}$$

$$3. \Delta G_{\text{reaction}} = \Delta H_{\text{reaction}} - T \cdot \Delta S_{\text{reaction}}$$

$$1. \Delta H_r = \Delta H^\circ_{\text{C}_6\text{H}_{12}\text{O}_6} + 6\Delta H^\circ_{\text{O}_2} - 6\Delta H^\circ_{\text{H}_2\text{O}} - 6\Delta H^\circ_{\text{CO}_2} = \dots \text{J/K/mol} \dots$$

$$\dots = -1263.78 - 6 \cdot 11.715 - (6 \cdot -285.85 + 6 \cdot -393.509) = -1334.07 + 4076154 = +2742.084 \text{ kJ/mol } \mathbf{endothermic} \dots$$

$$2. \Delta S_{\text{dispersed}} = -\Delta H_r / T = -2742.084 / 298.15 = -9196,995 \dots \text{J/K/mol} \dots$$

$$\Delta S_r = \Delta S^\circ_{\text{C}_6\text{H}_{12}\text{O}_6} + 6\Delta S^\circ_{\text{O}_2} - 6\Delta S^\circ_{\text{H}_2\text{O}} - 6\Delta S^\circ_{\text{CO}_2} = \dots \text{J/mol/K} \dots$$

$$\dots = 269.45 + 6 \cdot 110.876 - (6 \cdot 69.9565 + 6 \cdot 213.74) = 934.706 - 1702.179 = -767.473 \text{ J/mol/K} \dots$$

$$3. \Delta S_{\text{total}} = \Delta S_r + \Delta S_{\text{dispersed}} = -767.473 - 9196,9948 = -9964,4678 \dots \text{J/K/mol} \dots$$

$$\Delta G_r = \Delta H_r - T \cdot \Delta S_r = +2742.084 - 298.15 \cdot -767.473 = +3942.084 + 228.822 = +2970.906 \mathbf{endoergic} \dots$$

$$\dots \text{J/K/mol} \dots$$

$$T \cdot \Delta S_{\text{total}} = -9964,4678 \cdot 298,15 = \mathbf{-2970.9} \dots \text{kJ/mol} \dots$$

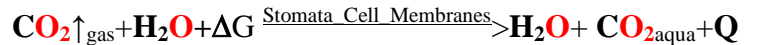
bound $T\Delta S_{\text{total}} \leftarrow$ accumulate energy $\Delta G_{\text{reversereaction}} \leftarrow Q = -2742.084 \text{ kJ/mol}$ **not spontaneous** $\Delta G_{\text{reaction}} = +2970,906 \text{ kJ/mol} \dots$

THERMODYNAMICS Exercise II CO₂ gas assimilation in water CO_{2(aqua)} reaction

Calculate ΔH_r, ΔS_r, ΔG_r at standard conditions 298.15 K. Reaction is **exothermic**, **athermic**, **endothermic**? From CO₂ gas assimilation in water CO_{2(aqua)} reaction for green plants +stomata enclosed surface of cell membranes on photosynthetic reaction center PRC+h•v using the data table! Mention whether the reaction will be **exoergic** or **endoergic**!

Initial compounds => products

Substance	ΔH _r ^o , kJ/mol	ΔS _r ^o , J/mol/K	ΔG _r ^o , kJ/mol
CO _{2(aqua)}	-413,7076	117,57	-385,98
H ₂ O	-285,85	69,9565	-237,191
CO _{2↑gas}	-393,509	213,74	-394,359



1. ΔH_{reaction} = ΣΔH_{products}^o - ΣΔH_{initial compounds}^o

2. ΔS_{reaction} = ΣΔS_{products}^o - ΣΔS_{initial compounds}^o

3. ΔG_{reaction} = ΔH_{reaction} - T•ΔS_{reaction}

1. ΔH_r=ΔH_{H2O}^o+ ΔH_{CO2aqua}^o-ΔH_{H2O}^o-ΔH_{CO2gas}^o=.....kJ/mol.....
=-413,7076-285,85-(-393,509+-285,85)=-413,7076-(-393,509) = -20,1986 kJ/mol **exothermic**.....

ΔS_{dispersed}= - ΔH_r/ T =20,1986/298.15= 67,746436J/K/mol.....

2. ΔS_r=ΔS_{H2O}^o+ ΔS_{CO2aqua}^o-ΔS_{H2O}^o-ΔS_{CO2gas}^o=.....J/mol/K.....
=117,57+69,9565-(213,74+69,9565)= 117,57-(-213,74)= -96,17.....J/mol/K.....

ΔS_{total}= ΔS_r+ ΔS_{dispersed}=-96,17 +67,746436 = -28,424
J/K/mol.....

3. ΔG_r = ΔH_r - T*ΔS_r = -20,1986-298.15*-96,17= -20,1986+28.673 = +8,474
kJ/mol.....
**endoergic**.....

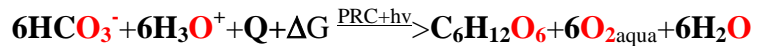
T•ΔS_{total}=-28,424*298,15K=-8,47.....kJ/mol.....

bound TΔS_n← accumulate energy ΔG_{reversereaction}←.Q=-3942.084 kJ/mol..**not spontaneous** ΔG_{reaction} = +8,474kJ/mol

THERMODYNAMICS Exercise III Bicarbonate 6HCO_3^- photosynthesis to 6O_2 and $\text{C}_6\text{H}_{12}\text{O}_6$

Calculate ΔH_r , ΔS_r , ΔG_r . Reaction is **exothermic**, **athermic**, **endothermic**? From water, Bicarbonate assimilation reaction in green plants with blue and red photon $E=h\nu$ absorption photosynthesis in photosynthetic reaction center PRC+ $h\nu$ for $6\text{O}_{2\text{aqua}}$ and $\text{C}_6\text{H}_{12}\text{O}_6$ at standard conditions 298.15 K using the data table! Mention whether the reaction will be **exoergic** or **endoergic**!

Initial compounds => products glucose + oxygen + water



<biooxidation (Krebs cycle, Glycolyse)

$$1. \Delta H_{\text{reaction}} = \sum \Delta H^\circ_{\text{products}} - \sum \Delta H^\circ_{\text{initial compounds}}$$

$$2. \Delta S_{\text{reaction}} = \sum \Delta S^\circ_{\text{products}} - \sum \Delta S^\circ_{\text{initial compounds}}$$

$$3. \Delta G_{\text{reaction}} = \Delta H_{\text{reaction}} - T \cdot \Delta S_{\text{reaction}}$$

Substance	$\Delta H^\circ_r, \text{kJ/mol}$	$\Delta S^\circ_r, \text{J/mol/K}$
$\text{C}_6\text{H}_{12}\text{O}_6(\text{aq})$	-1263,78	269,45
$\text{O}_{2\text{aqua}}$	-11,715	110,876
H_2O	-285,85	69,9565
H_3O^+	-285,81	-3,854
HCO_3^-	-689,93	98,324

$$1. \Delta H_r = \Delta H^\circ_{\text{C}_6\text{H}_{12}\text{O}_6} + 6\Delta H^\circ_{\text{O}_2} + 6\Delta H^\circ_{\text{H}_2\text{O}} - 6\Delta H^\circ_{\text{H}_3\text{O}^+} - 6\Delta H^\circ_{\text{HCO}_3^-} = +2805,27 \text{ kJ/mol} \dots$$

$$\dots = 6 \cdot (-689,93) + 6 \cdot (-11,715) - (-1263,78 - 6 \cdot 11,715 - 6 \cdot 285,85) = -3049,17 + 5854,44 = +2805,27 \text{ kJ/mol} \text{ **endothermic** \dots}$$

$$2. \Delta S_{\text{dispersed}} = -\Delta H_r / T = -2805,27 \cdot 1000 / 298,15 = -9408,9217 \text{ J/K/mol} \dots$$

$$\Delta S_r = \Delta S^\circ_{\text{C}_6\text{H}_{12}\text{O}_6} + 6\Delta S^\circ_{\text{O}_2} + 6\Delta S^\circ_{\text{H}_2\text{O}} - 6\Delta S^\circ_{\text{H}_3\text{O}^+} + 6\Delta S^\circ_{\text{HCO}_3^-} = \dots \text{ J/mol/K} \dots$$

$$\dots = 6 \cdot 98,324 + 6 \cdot (-3,854) - (269,45 + 6 \cdot 110,876 + 6 \cdot 69,9565) = 566,82 - 1354,45 = -787,625 \text{ J/mol/K} \dots$$

$$\Delta S_{\text{total}} = \Delta S_r + \Delta S_{\text{dispersed}} = -787,625 - 9408,9217 = -10196,55 \text{ J/K/mol} \dots$$

$$3. \Delta G_r = \Delta H_r - T \cdot \Delta S_r = +2805,27 - 298,15 \cdot (-0,787625) = +2805,27 + 247,0669 = 3040,1 \text{ kJ/mol} \dots$$

... **endoergic**...

$$T \cdot \Delta S_{\text{total}} = -10196,55 \text{ J/mol} \cdot 298,15 \text{ K} = -3040,1 \text{ kJ/mol} \dots$$

bound $T \Delta S_{\text{total}} \leftarrow$ accumulate energy $\Delta G_{\text{reverse reaction}} \leftarrow \dots$ $Q = -2805,27 \text{ kJ/mol}$ **not spontaneous** $\Delta G^\circ_{\text{reaction}} = +3040,1 \text{ kJ/mol} \dots$

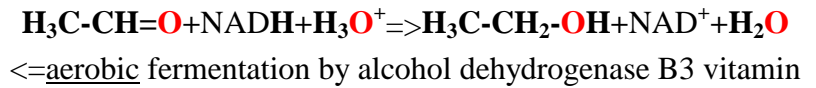
p.3: <http://aris.gusc.lv/BioThermodynamics/BioChemicalProcesE.pdf>.

accumulate energy $T \Delta S_{\text{total}} = -3040,1 \text{ kJ/mol}$ is bound in products: $\text{C}_6\text{H}_{12}\text{O}_6 + 6\text{O}_{2\text{aqua}} + 6\text{H}_2\text{O} \dots$

THERMODYNAMICS Exercise IV Vitamin B3 etanal $\text{H}_3\text{C}-\text{CH}=\text{O}$ reducing to ethanol $\text{H}_3\text{C}-\text{CH}_2-\text{OH}$ product

Calculate ΔH_r , ΔS_r , ΔG_r at standard conditions 298.15 K . Reaction is **exothermic** , **athermic** , **endothermic**?
 Vitamin B3 for anaerobic ethanal reduction to ethanol product with alcohol dehydrogenase using the data table!
 Mention whether the reaction will be **exoergic** or **endoergic**! Initial compounds => products+ ΔG + Q

Substance	ΔH_r° , kJ/mol	ΔS_r° , J/mol/K
$\text{H}_3\text{C}-\text{CH}=\text{O}_{aq}$	-212,23	-281,84
$\text{NADH}_{(aq)}$	-1036,66	-140,50
$\text{H}_3\text{O}^+_{(aq)}$	-285.81	-3,854
$\text{H}_3\text{C}-\text{CH}_2-\text{OH}_{aq}$	-288,3	-357,74
$\text{NAD}^+_{(aq)}$	-1007,48	-183
$\text{H}_2\text{O}_{(aq)}$	-285.85	69,96



1. $\Delta H_{\text{reaction}} = \Sigma \Delta H^\circ_{\text{products}} - \Sigma \Delta H^\circ_{\text{initial compounds}}$
 2. $\Delta S_{\text{reaction}} = \Sigma \Delta S^\circ_{\text{products}} - \Sigma \Delta S^\circ_{\text{initial compounds}}$
 3. $\Delta G_{\text{reaction}} = \Delta H_{\text{reaction}} - T \cdot \Delta S_{\text{reaction}}$

1. $\Delta H_r = \Delta H^\circ_{\text{CH}_3\text{CH}_2\text{OH}} + \Delta H^\circ_{\text{H}_2\text{O}} + \Delta H^\circ_{\text{NAD}^+} - \Delta H^\circ_{\text{H}_3\text{O}^+} - \Delta H^\circ_{\text{CH}_3\text{CHO}} - \Delta H^\circ_{\text{NADH}} = \dots \text{kJ/mol} \dots$
 $\dots = -288,3 - 1007,48 - 285,85 - (-212,23 - 1036,66 - 285,81) = -1581,63 + 1534,7 = -46,93 \text{ kJ/mol}$ **exothermic**...

2. $\Delta S_{\text{dispersed}} = -\Delta H_r / T = -(-46,93) / 298,15 = +157,4 \dots \text{J/K/mol} \dots$

$\Delta S_r = \Delta S^\circ_{\text{CH}_3\text{CH}_2\text{OH}} + \Delta S^\circ_{\text{H}_2\text{O}} + \Delta S^\circ_{\text{NAD}^+} - \Delta S^\circ_{\text{H}_3\text{O}^+} - \Delta S^\circ_{\text{CH}_3\text{CHO}} - \Delta S^\circ_{\text{NADH}} = \dots \text{J/K/mol} \dots$
 $\dots = -357,7394 - 183 + 69,956 - (-281,838 - 140,50 - 3,854) = -470,78 + 426,192 = -44,588 \text{ J/mol/K} \dots$

3. $\Delta S_{\text{total}} = \Delta S_r + \Delta S_{\text{dispersed}} = 157,4 - 44,588 = +112,812 \dots \text{J/K/mol} \dots$

$\Delta G_r = \Delta H_r - T \cdot \Delta S_r = -46,93 - 298,15 \cdot (-44,588) / 1000 = -33,636 \dots \text{kJ/mol} \dots$
 ... **exoergic**...

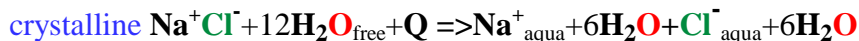
$T \cdot \Delta S_{\text{total}} = +112,812 \text{ J/K/mol} \cdot 298,15 \text{ K} = +33,635 \dots \text{kJ/mol} \dots$

bound $T \Delta S_{\text{total}} \leftarrow$ lost energy $\Delta G_{\text{reversereaction}} \leftarrow \dots Q = +46,93 \text{ kJ/mol}$ **spontaneous** $\Delta G_{\text{reaction}} = -33,636 \text{ kJ/mol} \dots$

Calculate ΔH_r , ΔS_r , ΔG at standard conditions 298.15 K. Reaction is **exothermic**, **athermic**, **endothermic**? For **crystalline** salt **Na⁺Cl⁻** hydration reaction with water using the data table! Mention whether the reaction will be **exoergic** or **endoergic**!

Initial compounds => products

Substance	$\Delta H_r^\circ, \text{kJ/mol}$	$\Delta S_r^\circ, \text{J/mol/K}$
crystalline Na⁺Cl⁻	-411.12	72.00
Na⁺_{aqua}	-240.10	59.00
Cl⁻_{aqua}	-167.2	56.50



1. $\Delta H_{\text{reaction}} = \Sigma \Delta H^\circ_{\text{products}} - \Sigma \Delta H^\circ_{\text{initial compounds}}$

2. $\Delta S_{\text{reaction}} = \Sigma \Delta S^\circ_{\text{products}} - \Sigma \Delta S^\circ_{\text{initial compounds}}$

3. $\Delta G_{\text{reaction}} = \Delta H_{\text{reaction}} - T \cdot \Delta S_{\text{reaction}}$

1. $\Delta H_r = \Delta H^\circ_{\text{Na}^+} + \Delta H^\circ_{\text{Cl}^-} - \Delta H^\circ_{\text{Na}^+\text{Cl}^-} = \dots \text{kJ/mol} \dots$
 $\dots = -240.1 - 167.2 - (-411.12) = -407.3 + 411.12 = +3.82 \text{ kJ/mol}$ **endothermic** \dots

2. $\Delta S_{\text{dispersed}} = -\Delta H_r / T = -3.82 / 298.15 = -12.812 \dots \text{J/mol/K} \dots$

2. $\Delta S_r = \Delta S^\circ_{\text{Na}^+} + \Delta S^\circ_{\text{Cl}^-} - \Delta S^\circ_{\text{Na}^+\text{Cl}^-} = 59.00 + 56.50 - (72.00) = 115.5 - 72.00 = +43.5 \dots \text{J/mol/K} \dots$

3. $\Delta S_{\text{total}} = \Delta S_r + \Delta S_{\text{dispersed}} = -12.812 + 43.5 = +30.688 \dots \text{J/mol/K} \dots$

3. $\Delta G_r = \Delta H_r - T \cdot \Delta S_r = +3.82 - 298.15 \cdot 0.0435 = -9.15 \dots \text{kJ/mol} \dots$
exoergic \dots

3. $T \cdot \Delta S_{\text{total}} = +30.688 \text{ J/mol/K} \cdot 298.15 \text{ K} = +9.15 \dots \text{kJ/mol} \dots$

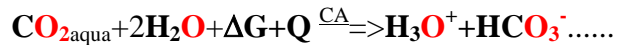
bound $T \Delta S_{\text{total}} \leftarrow$ lost free energy $\Delta G_{\text{reversereaction}} \leftarrow \dots Q = -3.82 \text{ kJ/mol} \dots$ **spontaneous** $\Delta G_r = -9.15 \text{ kJ/mol}$ \dots

THERMODYNAMICS Exercise VI Carbonic Anhydrase made acid/base equilibrium $\text{H}_2\text{O}^{\text{CA}}/\text{CO}_2/\text{H}_3\text{O}^++\text{HCO}_3^-$

Calculate ΔH_r , ΔS_r , ΔG at standard conditions (298.15 K). Reaction is **exothermic**, **athermic**, **endothermic**? For the Enzyme Carbonic anhydrase (CA) made acid/base equilibrium $\text{H}_2\text{O}^{\text{CA}}/\text{CO}_2/\text{H}_3\text{O}^++\text{HCO}_3^-$ using CA driven reaction of aqua CO_2 with water molecules $2\text{H}_2\text{O}$ using data table! Will be **exoergic** or **endoergic**!

Initial compounds => products

Substance	ΔH_f° , kJ/mol	ΔS_f° , J/mol/K
H_3O^+	-285.81	-3.854
HCO_3^-	-689.93	98.324
H_2O	-285.85	69.9565
$\text{CO}_{2\text{aqua}}$	-413.7976	117.5704



1. $\Delta H_{\text{reaction}} = \Delta H^\circ_{\text{products}} - \Delta H^\circ_{\text{initial compounds}}$

2. $\Delta S_{\text{reaction}} = \Delta S^\circ_{\text{products}} - \Delta S^\circ_{\text{initial compounds}}$

3. $\Delta G_{\text{reaction}} = \Delta H_{\text{reaction}} - T \cdot \Delta S_{\text{reaction}}$

1. $\Delta H_r = \Delta H^\circ_{\text{H}_3\text{O}^+} + \Delta H^\circ_{\text{HCO}_3^-} - 2\Delta H^\circ_{\text{H}_2\text{O}} - \Delta H^\circ_{\text{CO}_2} = \dots\dots\dots$

$= -285.81 - 689.93 - (2 \cdot -285.85 - 413.7976) = -975.74 + 985.3276 = +9.7576$ **endothermic**.....

.....
.....
.....
.....
.....

$\Delta S_{\text{dispersed}} = -\Delta H_r / T = -9.7576 / 298.15 = -32.727$ kJ/mol.....
..... J/K/mol.....

.....
.....
.....
.....
.....

2. $\Delta S_r = \Delta S^\circ_{\text{H}_3\text{O}^+} + \Delta S^\circ_{\text{HCO}_3^-} - 2\Delta S^\circ_{\text{H}_2\text{O}} - \Delta S^\circ_{\text{CO}_2} = \dots\dots\dots$ J/mol/K.....
.....
..... $= -3.854 + 98.324 - (2 \cdot 69.9565 + 117.5704) = 94.47 - 257.482 = -163.0134$ J/mol/K.....

.....
.....
.....
.....
.....

$\Delta S_{\text{total}} = \Delta S_r + \Delta S_{\text{dispersed}} = -32.727 - 163.0134 = -195.169$ J/K/mol.....

.....
.....
.....
.....
.....

3. $\Delta G_r = \Delta H_r - T \cdot \Delta S_r = +9.7576 + 298.15 \cdot 0.1630134 = +58.19$ **endoergic**..... kJ/mol.....

.....
.....
.....
.....
.....

$T \cdot \Delta S_{\text{total}} = -195.7404 \cdot 298.15 \text{ K} = -58.19$ kJ/mol.....

bound $T \Delta S_n \leftarrow$ accumulated free energy $\Delta G_{\text{reverse reaction}} \leftarrow$ $Q = -9.7576$ kJ/mol **endoergic** $\Delta G_r_{\text{reaction}} = +58.19$ kJ/mol.....

THERMODYNAMICS Exercise VII $\text{H}_2\text{O} + \text{CO}_2$ using ionic channels drive reaction $\text{H}_3\text{O}^+ + \text{HCO}_3^-$ to gas CO_2

Calculate ΔH_r , ΔS_r , ΔG at standard conditions (298.15 K). Acid/base equilibrium $\text{H}_2\text{O} + \text{CO}_2$ using proton and ionic channels drive reaction in lungs $\text{H}^+ + \text{HCO}_3^-$ to breath out gas CO_2 with water $2\text{H}_2\text{O}$ (**exothermic, athermic or endothermic?**). To use data table! Will be **exoergic or endoergic!**

Substance	ΔH_r° , kJ/mol	ΔS_r° , J/mol/K
H_3O^+	-285.81	-3.854
HCO_3^-	-689.93	98.324
H_2O	-285.85	69.9565
$\text{CO}_2 \uparrow_{\text{gas}}$	-393,509	213,74

Initial compounds $\text{H}_3\text{O}^+ + \text{HCO}_3^- + \text{Q} \Rightarrow \text{CO}_2_{\text{gas}} + 2\text{H}_2\text{O} + \Delta G$

\Leftarrow assimilation for photosynthesis in plant stomata cells

1. $\Delta H_{\text{reaction}} = \Delta H^\circ_{\text{products}} - \Delta H^\circ_{\text{initial compounds}}$

2. $\Delta S_{\text{reaction}} = \Delta S^\circ_{\text{products}} - \Delta S^\circ_{\text{initial compounds}}$

3. $\Delta G_{\text{reaction}} = \Delta H_{\text{reaction}} - T \cdot \Delta S_{\text{reaction}}$

1. $\Delta H_r = 2\Delta H^\circ_{\text{H}_2\text{O}} + \Delta H^\circ_{\text{CO}_2} - \Delta H^\circ_{\text{H}_3\text{O}} - \Delta H^\circ_{\text{HCO}_3} = \dots \text{kJ/mol} \dots$

.....

.....

.....

.....

.....

$\dots = 2 \cdot (-285,85) - 393,509 - (-285,81 - 689,93) = -965,209 + 975,74 = +10,531 \text{ kJ/mol}$ **endothermic**.....

$\Delta S_{\text{dispersed}} = -\Delta H_r / T = -10,531 / 298,15 = -35,3211 \dots \text{J/K/mol} \dots$

.....

.....

.....

.....

.....

.....

2. $\Delta S_r = 2\Delta S^\circ_{\text{H}_2\text{O}} + \Delta S^\circ_{\text{CO}_2} - \Delta S^\circ_{\text{H}_3\text{O}} - \Delta S^\circ_{\text{HCO}_3} = \dots \text{J/mol/K} \dots$

$\dots = 2 \cdot 69,9565 + 213,74 - (-3,854 + 98,324) = 353,653 - 94,47 = 259,183 \dots$

$\Delta S_{\text{total}} = \Delta S_r + \Delta S_{\text{dispersed}} = 259,183 - 35,3211 = +223,8619 \dots \text{J/K/mol} \dots$

.....

.....

.....

.....

.....

.....

3. $\Delta G_r = \Delta H_r - T \cdot \Delta S_r = 10,531 - 298,15 \cdot 0,259183 = -66,744411$ **exoergic**.....

$\dots \text{kJ/mol} \dots$

exoergic.....

.....

.....

.....

.....

$T \cdot \Delta S_{\text{total}} = 223,8619 \cdot 298,15 \text{ K} = +66,7444 \dots \text{kJ/mol} \dots$

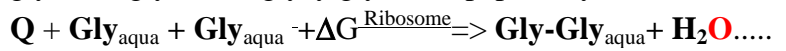
bound $T\Delta S_{\text{total}} \leftarrow$ lost free energy $\Delta G_{\text{reversereaction}} \leftarrow \dots \text{Q} = -10,531 \text{ kJ/mol}$ **exoergic spontaneous** $\Delta G_{\text{reaction}} = -66,7444 \text{ kJ/mol} \dots$

THERMODYNAMICS Exercise VIII glycine + glycine → glycyglycine dipeptide synthesis

Calculate ΔH_r , ΔS_r , ΔG_r at standard conditions (298.15 K). Reaction is **exothermic**, **athermic**, **endothermic**? For peptide synthesis polycondensation Enzyme ribosome governed reaction with amino acids glycine Gly (G) using the data table! Mention whether the reaction will be **exoergic** or **endoergic**!

..... J.Phys.Chem.Ref.Data, Vol. 19, No. 4, 1990; Chem. Phys. CRC, 2010-2005, p.876,882,1220,1223

glycine+ glycine → glycyglycine dipeptide synthesis



1. $\Delta H_{reaction} = \sum \Delta H^\circ_{products} - \sum \Delta H^\circ_{initial\ compounds}$

2. $\Delta S_{reaction} = \sum \Delta S^\circ_{p,products} - \sum \Delta S^\circ_{initial\ compounds}$

3. $\Delta G_{reaction, \text{ kJ/mol}} = \Delta H_{reaction} - T \cdot \Delta S_{reaction}$

$\Delta G^\circ_{formation} \text{ kJ/mol } \Delta G^\circ_{H_2O} = -237.19 \text{ kJ/mol}$

$Gly_{aqua} \Delta G_r = \sum \Delta G^\circ_{product} - \sum \Delta G^\circ_{initial_compounds}$

$Gly-Gly_{aqua} ; \Delta G_r = -200,5 - 213,275 - (2 \cdot -180,13) = -53.515 \dots$

H_2O ;

Viela	$\Delta H^\circ_r, \text{ kJ/mol}$	$\Delta S^\circ_r, \text{ J/mol/K}$
Gly_{aqua}	-554.56	76.45
$Gly-Gly_{aqua}$	-790.99	-1
H_2O	-285.83	69.9565
I=0 M	I=0,1 M	I=0.25 M
-180.13	-177.07.	-176.08
-200.55	-195.65	-194.07
-213.275	-213.275	213.275

$\Delta G_r = -195.65 - 213,275 - (2 \cdot -177.07) = -54,785 \text{ kJ/mol}$ **endoergic**.....

$\Delta G_r = -194,07 - 213,275 (2 \cdot -176,08) = -55,185 \text{ kJ/mol}$ **endoergic**.....

1. $\Delta H_r = \Delta H^\circ_{Gly-Gly} + \Delta H^\circ_{H_2O} - 2 \Delta H^\circ_{Gly} = -790.99 - 285.83 - (2 \cdot -554.56) = -1076.82 + 1109.12 = +32.3 \text{ kJ/mol}$ **endothermic**.....

2. $\Delta S_{dispersed} = -\Delta H_r / T = -32.3 / 298.15 = -108.335 \dots \text{ J/K/mol}$

$\Delta S_r = \Delta S^\circ_{Gly-Gly} + \Delta S^\circ_{H_2O} - 2 \Delta S^\circ_{Gly} = \dots \text{ J/mol/K}$
 $\dots = -1 + 69.9565 - (2 \cdot 76.45) = 68,957 - 152.9 = -83,944 \text{ J/mol/K} \dots$

3. $\Delta S_{total} = \Delta S_r + \Delta S_{dispersed} = -83,944 - 108,335 = -192,279 \dots \text{ J/K/mol}$

Page 3: <http://aris.gusc.lv/BioThermodynamics/08ThGlyGlyH2OCRC10sol.pdf>

$\Delta G_r = \Delta H_r - T \cdot \Delta S_r = 32,3 - 298,15 \cdot -0,083944 = 32,3 + 25,0279 = 57,328 \text{ kJ/mol}$ **endoergic**.....

ionic force is total ions summary concentration

$I = 1 \text{ mol/L (1 M)}$

for standart enthalpy $\Delta H^\circ_r, \text{ kJ/mol}$

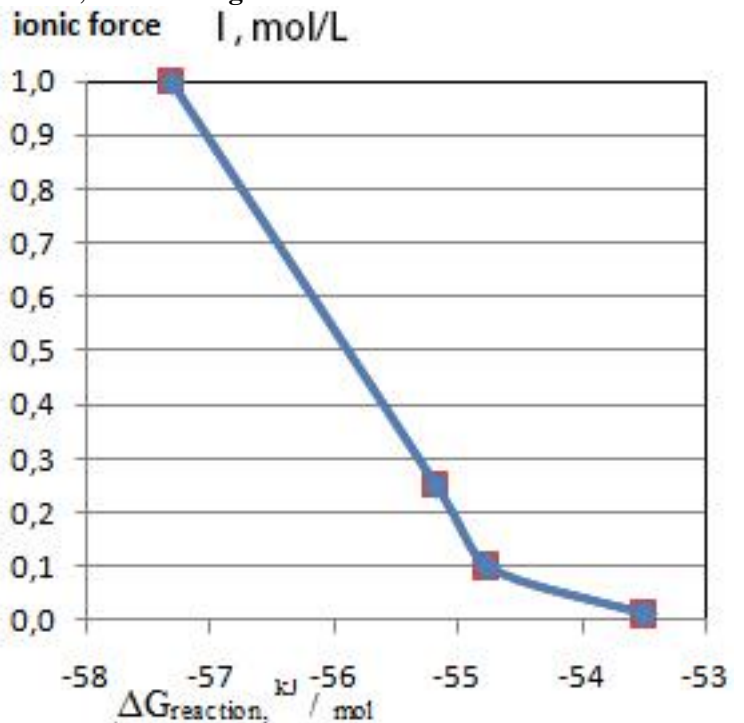
and

for standart entropy $\Delta S^\circ_r, \text{ J/mol/K}$

mesured values calculated

$\Delta G_r = 57 \text{ kJ/mol}$

Chem. Phys. CRC, 2010-2005, p.876,882,1220,1223



$T \cdot \Delta S_{total} = -192,279 \text{ J/K/mol} \cdot 298,15 \text{ K} = -57,328 \dots \text{ kJ/mol}$

bound $T \Delta S_n \leftarrow \text{lost free energy } \Delta G_{reversereaction} \leftarrow Q = -32.3 \dots \text{ kJ/mol}$ non spontaneous $\Delta G^\circ_{reaction} = 57,328 \dots \text{ kJ/mol}$

Calculate ΔH_r, ΔS_r, ΔG_r at standard conditions 298.15 K. Is **exothermic**, **athermic** or **endothermic**? Along concentration gradients through proton H⁺ channels [H₃O]_{right}/[H₃O]_{left} and through bicarbonate HCO₃⁻ channels [HCO₃]_{right}/[HCO₃]_{left} evaporation in lungs of water and CO₂ gas. To use the data table! Mention whether the reaction will be **exoergic** or **endoergic**! Initial compounds => products

Substance	ΔH _r ^o , kJ/mol	ΔS _r ^o , J/mol/K
H ₃ O ⁺	-285,81	-3,854
HCO ₃ ⁻	-689,93	98,324
H ₂ O	-285,85	69,9565
H ₂ O↑ _{gas}	-241,8352	188,7402
CO ₂ ↑ _{gas}	-393,509	213,74



$$1. \Delta H_{reaction} = \Sigma \Delta H^o_{products} - \Sigma \Delta H^o_{initial\ compounds}$$

$$2. \Delta S_{reaction} = \Sigma \Delta S^o_{products} - \Sigma \Delta S^o_{initial\ compounds}$$

$$3. \Delta G_{reaction} = \Delta H_{reaction} - T \cdot \Delta S_{reaction}$$

channels H⁺ : $\Delta G_H = RT \ln([H_3O]_{right}/[H_3O]_{left})$

channels HCO₃⁻ : $\Delta G_{HCO_3} = RT \ln([HCO_3]_{right}/[HCO_3]_{left})$

$$1. \Delta H_r = \Delta H^o_{H_2O} + \Delta H^o_{H_2O \uparrow_{gas}} + \Delta \Delta H^o_{CO_2} - \Delta H^o_{H_3O} - \Delta H^o_{HCO_3} = \dots\dots\dots \text{kJ/mol} \dots\dots$$

$$\dots = -285,85 - 241,8352 - 393,509 - (-285,81 - 689,93) = -921,19 + 975,74 = +54,546 \text{ kJ/mol } \mathbf{endothermic} \dots\dots \text{kJ/mol} \dots\dots$$

$$2. \Delta S_{dispersed} = -\Delta H_r / T = -54,546 / 298,15 = -182,9475 \dots\dots\dots \text{J/K/mol} \dots\dots$$

$$\Delta S_r = \Delta S^o_{H_2O} + \Delta S^o_{H_2O \uparrow_{gas}} + \Delta S^o_{CO_2} - \Delta S^o_{H_3O} - \Delta S^o_{HCO_3} = \dots\dots\dots \text{J/K/mol} \dots\dots$$

$$\dots\dots\dots = 69,956 + 188,74 + 213,74 - (-3,854 + 98,324) = 353,652 - 94,47 = +377,966 \text{ J/mol} \dots\dots$$

$$\Delta S_H = -R \ln(10^{-5,5} / 0,02754) = 75,42909 \text{ J/mol} \dots\dots \Delta S_{HCO_3} = -R \ln(0,0154 / 0,0338919) = 6,55847 \text{ J/mol} \dots\dots$$

$$\Delta S_{rH} = 377,966 + 75,42909 + 6,55847 = 459,954 \text{ J/mol} \dots\dots$$

$$3. \Delta S_{total} = \Delta S_r + \Delta S_{dispersed} = -182,95 + 377,966 = 195,016 \text{ J/K/mol} \dots\dots\dots$$

$$\Delta S_{Htotal} = \Delta S_{rH} + \Delta S_{dispersed} = -182,95 + 459,954 = 277,004 \text{ J/K/mol} \dots\dots\dots$$

$$\Delta G_r = \Delta H_r - T \cdot \Delta S_r = +54,546 - 298,15 \cdot 0,377966 = -58,144 \dots\dots\dots \text{kJ/mol} \dots\dots$$

$$\Delta G_H = RT \ln(10^{-5,5} / 0,02754) = -22,48918 \text{ kJ/mol} \dots\dots \Delta G_{HCO_3} = RT \ln(0,0154 / 0,0338919) = -1,9554 \text{ kJ/mol} \dots\dots$$

$$\Delta G_{rH} = \Delta H_r - T \cdot \Delta S_{rH} = +54,546 - 298,15 \cdot 0,459954 = -82,589 \dots\dots\dots \text{kJ/mol} \dots\dots$$

exoergic.....

$$T \cdot \Delta S_{total} = 195,016 \text{ J/K/mol} \cdot 298,15 \text{ K} = +58,144 \dots\dots\dots \text{kJ/mol} \dots\dots$$

$$T \cdot \Delta S_{Htotal} = 277,004 \text{ J/K/mol} \cdot 298,15 \text{ K} = -58,144 - 22,48918 - 1,9554 = +82,589 \text{ kJ/mol} \dots\dots\dots$$

bound TΔSn ← lost free energy ΔG_{reverse, reaction} ← Q = -54.546 kJ/mol. **spontaneous** ΔG_{reaction} = -58,14 kJ/mol...

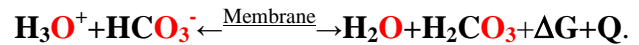
bound TΔSn ← lost free energy ΔG_{reverse, reaction} ← Q = -54.546 kJ/mol. **spontaneous** ΔG_{reaction} = -82,589 kJ/mol...

THERMODYNAMICS Exercise X. bicarbonate and proton on membrane *lung* epithelial cell surface **H₂CO₃**

Calculate ΔH_r , ΔS_r , ΔG_r at standard conditions 298.15 K. Reaction is **exothermic**, **athermic**, **endothermic**? For transfer bicarbonate and proton through channels on membrane from cell solution of *lung* to epithelial cell surface forming **H₂CO₃** using the data table! Mention whether the reaction will be **exoergic** or **anenergetic** or **endoergic**!

..... Initial compounds → products

Substance	ΔH_r° , kJ/mol	ΔS_r° , J/mol/K
H₃O⁺	-285.81	-3.854
HC₃O₃⁻	-689.93	98.324
H₂O	-285.85	69.9565
H₂CO₃	-699,65	187.00



1. $\Delta H_{\text{reaction}} = \sum \Delta H^\circ_{\text{products}} - \sum \Delta H^\circ_{\text{initial compounds}}$

2. $\Delta S_{\text{reaction}} = \sum \Delta S^\circ_{\text{products}} - \sum \Delta S^\circ_{\text{initial compounds}}$

3. $\Delta G_{\text{reaction}} = \Delta H_{\text{reaction}} - T \cdot \Delta S_{\text{reaction}}$

1. $\Delta H_r = \Delta H^\circ_{\text{H}_2\text{O}} + \Delta H^\circ_{\text{H}_2\text{CO}_3} - \Delta H^\circ_{\text{H}_3\text{O}} - \Delta H^\circ_{\text{HC}_3\text{O}_3} = \dots\dots\dots \text{kJ/mol} \dots$
 $= -285,85 - 699,65 - (-285,81 - 689,93) = -985,5 + 975,74 = -9.76 \text{ kJ/mol exothermic} \dots$

.....

$\Delta S_{\text{dispersed}} = - \Delta H_r / T = +9.76 / 298.15 = +32.735 \dots\dots\dots \text{J/K/mol} \dots$

.....

2. $\Delta S_r = \Delta S^\circ_{\text{H}_2\text{O}} + \Delta S^\circ_{\text{H}_2\text{CO}_3} - \Delta S^\circ_{\text{H}_3\text{O}} - \Delta S^\circ_{\text{HC}_3\text{O}_3} = \dots\dots\dots \text{J/mol/K} \dots$
 $\dots\dots\dots = 69,956 + 187 - (-3,854 + 98,324) = 256,956 - 94,47 = +162,486 \text{ J/mol/K} \dots\dots\dots$

.....

$\Delta S_{\text{total}} = \Delta S_r + \Delta S_{\text{dispersed}} = +32.735 + 162,486 = 195,221 \dots\dots\dots \text{J/K/mol} \dots$

.....

3. $\Delta G_r = \Delta H_r - T \cdot \Delta S_r = -9,76 - 298,15 \cdot 0,162486 = -58.2052 \dots\dots\dots \text{kJ/mol} \dots$
 **exoergic**

.....

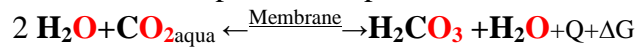
$T \cdot \Delta S_{\text{total}} = 195,221 \text{ J/K/mol} \cdot 298,15 \text{ K} = +58,2052 \dots\dots\dots \text{kJ/mol} \dots$
 bound $T \Delta S_n \leftarrow$ lost free energy $\Delta G_{\text{reversereaction}} \leftarrow Q = -9.76 \text{ kJ/mol} \dots$ **spontaneous** $\Delta G_{\text{reaction}} = -58.2 \text{ kJ/mol} \dots$

THERMODYNAMICS Exercise XI. $\text{CO}_{2\text{aqua}}$ two water molecules $2\text{H}_2\text{O}$ at *lung* epithelial cell surface H_2CO_3

Calculate ΔH_r , ΔS_r , ΔG_r at standard conditions 298.15 K. Reaction is **exothermic**, **athermic**, **endothermic**? For carbon dioxide water solution driven reaction of aqua CO_2 with water molecules $2\text{H}_2\text{O}$ at *lung* epithelial cell surface forming H_2CO_3 ! Mention reaction will be **exoergic** or **anenergetic** or **endoergic**!

Substance	ΔH_r° , kJ/mol	ΔS_r° , J/mol/K
$\text{CO}_{2\text{aqua}}$	-413.7976	117.5704
H_2O	-285.85	69.9565
H_2CO_3	-699,65	187.00

Initial compounds → products



1. $\Delta H_{\text{reaction}} = \sum \Delta H^\circ_{\text{products}} - \sum \Delta H^\circ_{\text{initial compounds}}$

2. $\Delta S_{\text{reaction}} = \sum \Delta S^\circ_{\text{products}} - \sum \Delta S^\circ_{\text{initial compounds}}$

3. $\Delta G_{\text{reaction}} = \Delta H_{\text{reaction}} - T \cdot \Delta S_{\text{reaction}}$

1. $\Delta H_r = \Delta H^\circ_{\text{H}_2\text{O}} + \Delta H^\circ_{\text{H}_2\text{CO}_3} - 2\Delta H^\circ_{\text{H}_2\text{O}} - \Delta H^\circ_{\text{CO}_{2\text{aqua}}} = \dots \text{kJ/mol} \dots$
 $= -285.85 - 699,65 - (2 \cdot -285.81 - 413,7976) = -985.5 + 985.418 = -0,0824 \text{ kJ/mol}$ **athermic**.....

.....

$\Delta S_{\text{dispersed}} = -\Delta H_r / T = +0,0824 / 298.15 = +0,27637 \dots \text{J/K/mol} \dots$

.....

2. $\Delta S_r = \Delta S^\circ_{\text{H}_2\text{O}} + \Delta S^\circ_{\text{H}_2\text{CO}_3} - 2\Delta S^\circ_{\text{H}_2\text{O}} - \Delta S^\circ_{\text{CO}_{2\text{aqua}}} = \dots \text{J/K/mol} \dots$
 $= 69.956 + 187 - (117,5704 + 2 \cdot 69.956) = 256,956 - 257,4824 = -0,5264 \text{ J/mol/K} \dots$

.....

$\Delta S_{\text{total}} = \Delta S_r + \Delta S_{\text{dispersed}} = -0,5264 + 0,27637 = -0,25 \dots \text{J/K/mol} \dots$

.....

$\Delta G_r = \Delta H_r - T \cdot \Delta S_r = -0,0824 - 298.15 \cdot -0,0005264 = 0,07455 \dots \text{kJ/mol} \dots$
anenergetic.....

.....

$T \cdot \Delta S_{\text{total}} = -0,25 \text{ J/K/mol} \cdot 298,15 \text{ K} = -0,0745 \dots \text{kJ/mol} \dots$

bound $T \Delta S_n \leftarrow$ accumulate free energy $\Delta G_{\text{reversereaction}} \leftarrow Q = +0,0824 \text{ kJ/mol} \dots$ **anenergetic** $\Delta G_{\text{reaction}} = +0,0745 \text{ kJ/mol} \dots$

THERMODYNAMICS Exercise XII. H_2CO_3 decomposition CO_2 gas H_2O at *lung* epithelial cell surface

Calculate ΔH_r , ΔS_r , ΔG_r at standard conditions 298.15 K. Reaction is **exothermic**, **athermic**, **endothermic**? From water carbonic acid H_2CO_3 decomposition reaction to carbon dioxide CO_2 gas and water H_2O at *lung* epithelial cell surface from H_2CO_3 using the data table! Mention whether the reaction will be **exoergic** or **endoergic**!

..... Initial compounds => products

Substance	$\Delta H_r^\circ, \text{kJ/mol}$	$\Delta S_r^\circ, \text{J/mol/K}$
$\text{CO}_2 \uparrow_{\text{gas}}$	-393,509	213,74
H_2O	-285,85	69,9565
H_2CO_3	-699,65	187,00



1. $\Delta H_{\text{reaction}} = \sum \Delta H^\circ_{\text{products}} - \sum \Delta H^\circ_{\text{initial compounds}}$

2. $\Delta S_{\text{reaction}} = \sum \Delta S^\circ_{\text{products}} - \sum \Delta S^\circ_{\text{initial compounds}}$

3. $\Delta G_{\text{reaction}} = \Delta H_{\text{reaction}} - T \cdot \Delta S_{\text{reaction}}$

1. $\Delta H_r = \Delta H^\circ_{\text{H}_2\text{O}} + \Delta H^\circ_{\text{CO}_2} - \Delta H^\circ_{\text{H}_2\text{CO}_3} = \dots \text{kJ/mol} \dots$
 $\dots = -285,85 - 393,509 - (-699,65) = -679,359 + 699,65 = +20,291 \text{ kJ/mol}$ **endothermic**.....

$\Delta S_{\text{dispersed}} = -\Delta H_r / T = -20,291 / 298,15 = -68,056 \dots \text{J/K/mol} \dots$

2. $\Delta S_r = \Delta S^\circ_{\text{H}_2\text{O}} + \Delta S^\circ_{\text{CO}_2} - \Delta S^\circ_{\text{H}_2\text{CO}_3} = \dots \text{J/K/mol} \dots$
 $\dots = 69,956 + 213,74 - (187) = 257,482 - 187 = +70,482 \text{ J/mol/K} \dots$

$\Delta S_{\text{total}} = \Delta S_r + \Delta S_{\text{dispersed}} = -68,056 + 70,482 = 2,426 \dots \text{J/K/mol} \dots$

3. $\Delta G_r = \Delta H_r - T \cdot \Delta S_r = +20,291 - 298,15 \cdot 0,070482 = -8,538912 \dots \text{kJ/mol} \dots$
exoergic.....

$T \cdot \Delta S_{\text{total}} = 2,426 \text{ J/K/mol} \cdot 298,15 \text{ K} = +723,3 \dots \text{kJ/mol} \dots$

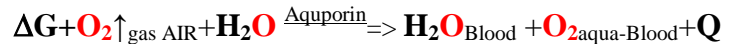
bound $T \Delta S_{\text{total}} \leftarrow$ lost free energy $\Delta G_{\text{reversereaction}} \leftarrow Q = -20,291 \text{ kJ/mol}$ **spontaneous** $\Delta G_{\text{reaction}} = -8,539 \text{ kJ/mol} \dots$

THERMODYNAMICS Exercise XIII. O_2 ↑gas respiration through membrane aquaporins to form $O_{2\text{aqua-Blood}}$

Calculate ΔH_r , ΔS_r , ΔG_r at standard conditions 298.15 K using the data table! Reaction is **exothermic**, **athermic**, **endothermic**? AIR O_2 ↑gas assimilation reaction for human body respiration through membrane aquaporins to form $O_{2\text{aqua-Blood}}$! Mention whether the reaction will be **exoergic** or **endoergic**!

Initial compounds => products

Substance	ΔH_f° , kJ/mol	ΔS_f° , J/mol/K
$O_{2\text{aqua}}$	-11,715	110,876
H_2O	-285,85	69,9565
O_2 ↑gas	0,0	205,04



$$1. \Delta H_{\text{reaction}} = \sum \Delta H^\circ_{\text{products}} - \sum \Delta H^\circ_{\text{initial compounds}}$$

$$2. \Delta S_{\text{reaction}} = \sum \Delta S^\circ_{\text{products}} - \sum \Delta S^\circ_{\text{initial compounds}}$$

$$3. \Delta G_{\text{reaction}} = \Delta H_{\text{reaction}} - T \cdot \Delta S_{\text{reaction}}$$

$$\Delta H_r = \Delta H^\circ_{H_2O} + \Delta H^\circ_{O_{2\text{aqua-Blood}}} - \Delta H^\circ_{H_2O} - \Delta H^\circ_{O_2\text{gas-AIR}} = \dots \text{kJ/mol} \dots$$

$$\dots = (-285,85 + -11,715) - (-285,85 + 0,0) = -285,85 - 11,715 + 285,85 = -11,715 \text{ kJ/mol} \text{ exothermic} \dots$$

$$\Delta S_{\text{dispersed}} = -\Delta H_r / T = 11,715 / 298,15 = +39,292 \dots \text{J/K/mol} \dots$$

$$\dots = 110,876 + 69,9565 - (69,9565 + 205,04) = 110,876 - 205,04 = -94,164 \text{ J/mol} \dots$$

$$2. \Delta S_r = \Delta S^\circ_{H_2O} + \Delta S^\circ_{O_{2\text{aqua-Blood}}} - \Delta S^\circ_{H_2O} - \Delta S^\circ_{O_2\text{gas-AIR}} = \dots \text{J/K/mol} \dots$$

$$\dots = 69,9565 + 110,876 - (205,04 + 69,9565) = 180,83 - 274,997 = -94,164 \text{ J/mol} \dots$$

$$\Delta S_{\text{total}} = \Delta S_r + \Delta S_{\text{dispersed}} = -94,164 + 39,292 = -54,872 \dots \text{J/K/mol} \dots$$

$$3. \Delta G_r = \Delta H_r - T \cdot \Delta S_r = -11,715 + (298,15 \cdot 0,094164) = +11,715 - 19,1305 = +16,360 \dots \text{kJ/mol} \dots$$

endoergic.....

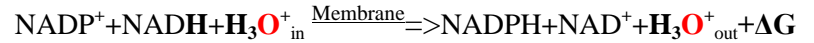
$$T \cdot \Delta S_{\text{total}} = -0,054872 \text{ kJ/K/mol} \cdot 298,15 \text{ K} = -16,36 \dots \text{kJ/mol} \dots$$

bound $T \Delta S_{\text{total}} \leftarrow$ accumulate energy $\Delta G_{\text{reversereaction}} \leftarrow Q = 11,715 \text{ kJ/mol}$ non-spontaneous **endoergic** $\Delta G_{\text{reaction}} = +16,36 \text{ kJ/mol} \dots$

THERMODYNAMICS Exercise XV. vitamin B3 $\text{H}_3\text{O}^+_{\text{in}}$ to $\text{H}_3\text{O}^+_{\text{out}}$ inter membrane space

Calculate ΔH_r , ΔS_r , ΔG_r at standard conditions 298.15 K using the data table! Reaction is **exothermic**, **athermic**, **endothermic**? For vitamin B3 reduced form NADH and oxidized form NADP^+ translocate hydrogen ions as protons through membrane from inner $\text{H}_3\text{O}^+_{\text{in}}$ to out side mitochondria $\text{H}_3\text{O}^+_{\text{out}}$ inter membrane space Reaction will be **exoergic** or **endoergic**!..... Initial compounds => products

Substance	ΔH°_r , kJ/mol	ΔS°_r , J/mol/K
NADP^+	-1007,48	577,897
$\text{NADH}_{(aq)}$	-1036,66	-140,50
$\text{H}_3\text{O}^+_{\text{out}}$	-285,81	-3,854
NADPH	-1036,66	763,005
$\text{NAD}^+_{(aq)}$	-1007,48	-183
$\text{H}_3\text{O}^+_{\text{in}}$	-285,81	-3,854



1. $\Delta H_{\text{reaction}} = \sum \Delta H^\circ_{\text{products}} - \sum \Delta H^\circ_{\text{initial compounds}}$

2. $\Delta S_{\text{reaction}} = \sum \Delta S^\circ_{\text{products}} - \sum \Delta S^\circ_{\text{initial compounds}}$

3. $\Delta G_{\text{reaction}} = \Delta H_{\text{reaction}} - T \cdot \Delta S_{\text{reaction}}$

Proton translocating transhydrogenase (EC1.6.1.1) ENZYME found in bacteria and animal mitochondria

that couples the transfer of reducing equivalents between

NAD(H) and NADP(H) to the translocation of protons across the membrane

1. $\Delta H_r = \Delta H^\circ_{\text{H}_3\text{O}^+_{\text{out}}} + \Delta H^\circ_{\text{NADPH}} + \Delta H^\circ_{\text{NAD}^+} - \Delta H^\circ_{\text{NADP}^+} - \Delta H^\circ_{\text{H}_3\text{O}^+_{\text{in}}} - \Delta H^\circ_{\text{NADH}} = \dots \text{kJ/mol} \dots$
 $\dots = -1036,66 - 1007,48 - 285,81 - (-1007,48 - 1036,66 - 285,81) = -2329,95 + 2329,95 = 0,0 \text{ kJ/mol}$ **athermic neutral**....

$\Delta S_{\text{dispersed}} = -\Delta H_r / T = -0 / 298,15 = +0,0 \dots \text{J/K/mol} \dots$

2. $\Delta S_r = \Delta S^\circ_{\text{H}_3\text{O}^+_{\text{out}}} + \Delta S^\circ_{\text{NADP}^+} + \Delta S^\circ_{\text{NADH}} - \Delta S^\circ_{\text{NADPH}} - \Delta S^\circ_{\text{H}_3\text{O}^+_{\text{in}}} - \Delta S^\circ_{\text{NAD}^+} = \dots \text{J/mol/K} \dots$
 $\dots = 763,005 - 183 - 3,854 - (577,897 - 140,50 - 3,854) = 576,2 - 433,543 = +142,6 \text{ J/mol/K} \dots$

$\Delta S_{\text{total}} = \Delta S_r + \Delta S_{\text{dispersed}} = 0,0 + 142,6 = +142,6 \dots \text{J/mol/K} \dots$

3. $\Delta G_r = \Delta H_r - T \cdot \Delta S_r = 0,0 - 298,15 \cdot (+142,6) / 1000 = -42,516 \dots \text{kJ/mol} \dots$
exoergic.....

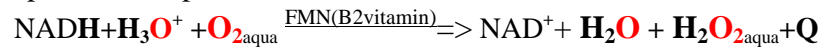
$T \cdot \Delta S_{\text{total}} = -142,6 \text{ J/mol} \cdot 298,15 \text{ K} = +42,516 \dots \text{kJ/mol} \dots$
 bound $T \Delta S_n \leftarrow$ lost energy for proton gradient $\leftarrow \text{H}^+_{\text{out}}$ $Q = +0,0 \text{ kJ/mol} \dots$ **spontaneous exoergic** $\Delta G_{\text{reaction}} = -42,516 \text{ kJ/mol} \dots$

THERMODYNAMICS Exercise XVI. $\text{NADH} + \text{H}_3\text{O}^+ + \text{O}_{2\text{aqua}} \xrightarrow{\text{FMN(B2vitamin)}} \text{NAD}^+ + \text{H}_2\text{O} + \text{H}_2\text{O}_{2\text{aqua}} + \text{Q}$

Calculate ΔH_r , ΔS_r , ΔG_r at standard conditions 298.15 K Reaction is **exothermic**, **athermic**, **endothermic** is **endoergic** or **exoergic**? For vitamin B3 reduced form NADH or NADPH flavin B2 vitamin FMN enzyme using oxygen $\text{O}_{2\text{aqua}}$ as electron acceptor for the oxidation of NADH with the production of hydrogen peroxide using the data table!

Initial compounds => products

Substance	ΔH_r° , kJ/mol	ΔS_r° , J/mol/K
$\text{O}_{2\text{aqua}}$	-11,715	110,876
$\text{NADH}_{(\text{aq})}$	-1036,66	-140,50
H_3O^+	-285,81	-3,854
H_2O	-285,85	69,9565
$\text{NAD}^+_{(\text{aq})}$	-1007,48	-183
$\text{H}_2\text{O}_{2\text{aqua}}$	-191,17	143,9



1. $\Delta H_{\text{reaction}} = \sum \Delta H^\circ_{\text{products}} - \sum \Delta H^\circ_{\text{initial compounds}}$

2. $\Delta S_{\text{reaction}} = \sum \Delta S^\circ_{\text{products}} - \sum \Delta S^\circ_{\text{initial compounds}}$

3. $\Delta G_{\text{reaction}} = \Delta H_{\text{reaction}} - T \cdot \Delta S_{\text{reaction}}$

NADH and NADPH oxidase (EC 1.6.99.1) ENZYME

$1 \Delta H_r = \Delta H^\circ_{\text{H}_2\text{O}_{2\text{aqua}}} + \Delta H^\circ_{\text{H}_2\text{O}} + \Delta H^\circ_{\text{NAD}^+} - \Delta H^\circ_{\text{H}_3\text{O}^+} - \Delta H^\circ_{\text{O}_{2\text{aqua}}} - \Delta H^\circ_{\text{NADH}} = \dots$

$\dots \Delta H_r = -1007,48 - 191,17 - 285,85 - (-1036,66 - 11,715 - 285,81) = -1484,5 + 1334,185 = -150,315 \text{ kJ/mol}$ **exothermic**..... kJ/mol.....

$\Delta S_{\text{dispersed}} = - \Delta H_r / T = +150,315 / 298.15 = +504,0416 \dots \text{J/K/mol} \dots$

2. $\Delta S_r = \Delta S^\circ_{\text{H}_2\text{O}_{2\text{aqua}}} + \Delta S^\circ_{\text{H}_2\text{O}} + \Delta S^\circ_{\text{NAD}^+} - \Delta S^\circ_{\text{H}_3\text{O}^+} - \Delta S^\circ_{\text{O}_{2\text{aqua}}} - \Delta S^\circ_{\text{NADH}} = \dots \text{J/mol/K} \dots$
 $\dots = -183 + 143,9 + 69,9565 - (110,876 - 140,50 - 3,854) = -39,1 - 29,624 = +64,335 \text{ J/mol/K} \dots$

3. $\Delta S_{\text{total}} = \Delta S_r + \Delta S_{\text{dispersed}} = +64,335 + 504,0416 = +568,3766 \dots \text{J/mol/K} \dots$

$\Delta G_r = \Delta H_r - T \cdot \Delta S_r = -150,315 - 298,15 \cdot (+64,335) / 1000 = -150,315 - 19,1815 = -169,5 \dots \text{kJ/mol} \dots$
exoergic.....

$T \cdot \Delta S_{\text{total}} = +568,3766 \text{ J/K/mol} \cdot 298,15 \text{ K} = +169,5 \dots \text{kJ/mol} \dots$

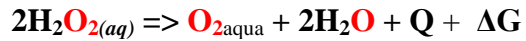
bound $T \Delta S_{\text{total}} \leftarrow$ lost energy \leftarrow $\text{NADH} + \text{O}_{2\text{aqua}} + \text{H}_3\text{O}^+ \cdot \text{Q} = +150,315 \text{ kJ/mol}$ **spontaneous exoergic** $\Delta G_{\text{reaction}} = -169,5 \text{ kJ/mol} \dots$

THERMODYNAMICS Exercise XVII Peroxide $2\text{H}_2\text{O}_2(aq)$ conversion to $\text{O}_2(aq) + 2\text{H}_2\text{O} + \text{Q}$

Calculate ΔH_r , ΔS_r , ΔG_r at standard conditions 298.15 K. Reaction is **exothermic**, **athermic**, **endothermic**? Peroxide $2\text{H}:\cdots\text{O}:-:\text{O}:\cdots\text{H}$ conversion to $\text{O}_2(aq) + 2\text{H}_2\text{O} + \text{Q}$ at human temperature (37 C) 310.15 K, using the data table! Mention whether the reaction will be **exoergic** or **endoergic**!

Initial compounds peroxide => products oxygen+water

Substance	ΔH_r° , kJ/mol	ΔS_r° , J/mol/K
$\text{H}_2\text{O}_2(aq)$	-191,17	143,9
$\text{O}_2(aq)$	-11,715	110,876
H_2O	-285,85	69,9565



$$1. \Delta H_{\text{reaction}} = \sum \Delta H^\circ_{\text{products}} - \sum \Delta H^\circ_{\text{initial compounds}}$$

$$2. \Delta S_{\text{reaction}} = \sum \Delta S^\circ_{\text{products}} - \sum \Delta S^\circ_{\text{initial compounds}}$$

$$3. \Delta G_{\text{reaction}} = \Delta H_{\text{reaction}} - T \cdot \Delta S_{\text{reaction}}$$

$$1. \Delta H_r = 2\Delta H^\circ_{\text{H}_2\text{O}} + \Delta H^\circ_{\text{O}_2} - 2\Delta H^\circ_{\text{H}_2\text{O}_2} = \dots \text{kJ/mol}$$

$$\dots = -11,715 - 2 \cdot 285,85 - (2 \cdot -191,17) = -133407583,4 + 383,415 = -201,08 \text{ kJ/mol } \mathbf{exothermic} \dots$$

.....
.....
.....
.....
.....

$$2. \Delta S_{\text{dispersed}} = -\Delta H_r / T = -(-201,08) / 310,15 = 648,33 \dots \text{J/K/mol} \dots$$

.....
.....
.....
.....
.....

$$\Delta S_r = 2\Delta S^\circ_{\text{H}_2\text{O}} + \Delta S^\circ_{\text{O}_2} - 2\Delta S^\circ_{\text{H}_2\text{O}_2} = \dots \text{J/mol/K}$$

$$\dots = 110,876 + 2 \cdot 69,9565 - (2 \cdot 143,9) = 250,789 - 287,8 = -37,011 \text{ J/mol/K} \dots$$

.....
.....
.....
.....
.....

$$3. \Delta S_{\text{total}} = \Delta S_r + \Delta S_{\text{dispersed}} = -37,011 + 648,33 = +611,319 \dots \text{J/mol/K}$$

.....
.....
.....
.....
.....

$$\Delta G_r = \Delta H_r - T \cdot \Delta S_r = -201,08 - 310,15 \cdot -0,037011 = -201,08 + 11,478962 = -189,601 \dots \text{kJ/mol}$$

.....**exoergic**.....

.....
.....
.....
.....
.....

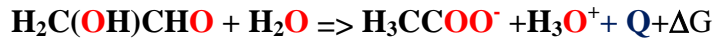
$$T \cdot \Delta S_{\text{total}} = 0,611319 \cdot 310,15 = +189,6 \dots \text{kJ/mol}$$

bound $T\Delta S_{\text{total}} \leftarrow$ accumulate energy $\Delta G_{\text{reversereaction}} \leq 0, Q = -201,08 \text{ kJ/mol } \mathbf{spontaneous} \Delta G_{\text{reaction}} = -189,6 \text{ kJ/mol} \dots$

THERMODYNAMICS Exercise XVIII Glyoxal $\text{H}_2\text{C}(\text{OH})\text{CHO}$ conversion to $\text{H}_3\text{CCOO}^- + \text{H}_3\text{O}^+ + \text{Q}$

Calculate ΔH_r , ΔS_r , ΔG_r at standard conditions 298.15 K. Reaction is **exothermic**, **athermic**, **endothermic**? Glyoxal $\text{H}_2\text{C}(\text{OH})\text{CHO}$ conversion to acetate $\text{H}_3\text{CCOO}^- + \text{H}_3\text{O}^+ + \text{Q}$ (25 C) 298.15 K, using the data table! Mention whether the reaction will be **exoergic** or **endoergic**!

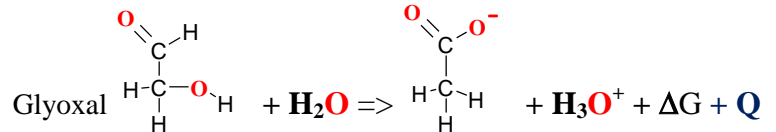
Substance	$\Delta H_r^\circ, \text{kJ/mol}$	$\Delta S_r^\circ, \text{J/mol/K}$
$\text{H}_2\text{C}(\text{OH})\text{CHO}$	-212	272,5
H_3CCOO^-	-486	85,3
$\text{H}_2\text{O}_{(aq)}$	-285,85	69,96
$\text{H}_3\text{O}^+_{(aq)}$	-285,81	-3,854



1. $\Delta H_{\text{reaction}} = \sum \Delta H^\circ_{\text{products}} - \sum \Delta H^\circ_{\text{initial compounds}}$

2. $\Delta S_{\text{reaction}} = \sum \Delta S^\circ_{\text{products}} - \sum \Delta S^\circ_{\text{initial compounds}}$

3. $\Delta G_{\text{reaction}} = \Delta H_{\text{reaction}} - T \cdot \Delta S_{\text{reaction}}$



1. $\Delta H_r = \Delta H^\circ_{\text{H}_3\text{CCOO}^-} + \Delta H^\circ_{\text{H}_3\text{O}^+} - \Delta H^\circ_{\text{H}_2\text{O}} + \Delta H^\circ_{\text{H}_2\text{C}(\text{OH})\text{CHO}} = \text{kJ/mol} \dots \dots \dots \text{kJ/mol} \dots \dots$
 $\dots \dots \dots = -486 - 285,81 - (-212 - 285,85) = -770,11 + 497,85 = -273,96 \text{ kJ/mol} \text{ exothermic} \dots$

2. $\Delta S_{\text{dispersed}} = - \Delta H_r / T = 273,96 / 298,15 = +918,966 \dots \dots \dots \text{J/K/mol} \dots \dots$

2. $\Delta S_r = \Delta S^\circ_{\text{CH}_3\text{COO}^-} + \Delta S^\circ_{\text{H}_3\text{O}^+} - \Delta S^\circ_{\text{H}_2\text{O}} - \Delta S^\circ_{\text{H}_2\text{C}(\text{OH})\text{CHO}} = \dots \dots \dots \text{J/mol/K} \dots \dots$
 $\dots \dots \dots = 85,3 - 3,854 - (69,96 + 272,5) = 81,446 - 342,46 = -261,014 \text{ J/mol/K} \dots \dots$

3. $\Delta S_{\text{total}} = \Delta S_r + \Delta S_{\text{dispersed}} = 918,966 - 261,014 = 657,952 \text{ J/mol/K} \dots \dots \dots \text{J/mol/K}$

4. $\Delta G_r = \Delta H_r - T \cdot \Delta S_r = -273,96 + 298,15 \cdot 0,261014 = -196,139 \dots \dots \dots \text{kJ/mol}$
 $\dots \dots \dots \text{exoergic} \dots \dots$

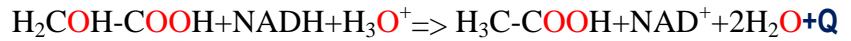
$T \cdot \Delta S_{\text{total}} = +657,952 \text{ J/mol} \cdot 298,15 \text{ K} = +196,168 \dots \dots \dots \text{kJ/mol} \dots$

bound $T \Delta S_{\text{total}} \leftarrow \text{lost energy } \Delta G_{\text{reversereaction}} \leftarrow \dots \text{Q} = +273,96 \text{ kJ/mol} \quad \text{spontaneous } \Delta G_{\text{reaction}} = -196,14 \text{ kJ/mol} \dots$

THERMODYNAMICS Exercise XIX Glycolic acid $\text{H}_2\text{COH-COOH}$ conversion to $\text{H}_3\text{C-COOH} + \text{Q}$

Calculate ΔH_r , ΔS_r , ΔG_r at standard conditions 298.15 K. Reaction is **exothermic**, **athermic**, **endothermic**? Glycolic acid $\text{H}_2\text{COH-COOH}$ conversion to acetate $\text{H}_3\text{C-COOH} + \text{Q}$ (25 C) 298.15 K, using the data table! Mention whether the reaction will be **exoergic** or **endoergic**!

Substance	$\Delta H_r^\circ, \text{kJ/mol}$	$\Delta S_r^\circ, \text{J/mol/K}$
$\text{H}_2\text{COH-COOH}$	-651	318,6
$\text{NADH}_{(aq)}$	-1036,66	-140,5
$\text{H}_3\text{O}^+_{(aq)}$	-285.81	-3,854
$\text{H}_3\text{C-COOH}$	-480.6	85.3
$\text{NAD}^+_{(aq)}$	-1007,48	-183
$\text{H}_2\text{O}_{(aq)}$	-285.85	69,96

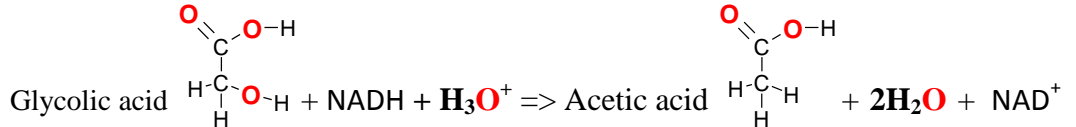


B3 vitamin \Rightarrow reduction

1. $\Delta H_{\text{reaction}} = \sum \Delta H^\circ_{\text{products}} - \sum \Delta H^\circ_{\text{initial compounds}}$

2. $\Delta S_{\text{reaction}} = \sum \Delta S^\circ_{\text{products}} - \sum \Delta S^\circ_{\text{initial compounds}}$

3. $\Delta G_{\text{reaction}} = \Delta H_{\text{reaction}} - T \cdot \Delta S_{\text{reaction}}$



1. $\Delta H_r = \Delta H^\circ_{\text{CH}_3\text{COOH}} + 2\Delta H^\circ_{\text{H}_2\text{O}} + \Delta H^\circ_{\text{NAD}^+} - \Delta H^\circ_{\text{H}_3\text{O}^+} - \Delta H^\circ_{\text{H}_2\text{COH-COOH}} - \Delta H^\circ_{\text{NADH}} = \text{kJ/mol} \dots \text{kJ/mol} \dots$
 $\dots = -480,6 - 1007,48 - 2 \cdot 285,85 - (-651 - 1036,66 - 285,81) = -2059,78 + 1973,47 = -86,31 \text{ kJ/mol}$ **exothermic**...

2. $\Delta S_{\text{dispersed}} = -\Delta H_r / T = -86,31 / 298,15 = +289,485 \dots \text{J/K/mol} \dots$

$\Delta S_r = \Delta S^\circ_{\text{CH}_3\text{COOH}} + 2\Delta S^\circ_{\text{H}_2\text{O}} + \Delta S^\circ_{\text{NAD}^+} - \Delta S^\circ_{\text{H}_3\text{O}^+} - \Delta S^\circ_{\text{H}_2\text{COH-COOH}} - \Delta S^\circ_{\text{NADH}} = \dots \text{J/K/mol} \dots$
 $\dots = 85,3 - 183 + 2 \cdot 69,956 - (318,6 - 140,50 - 3,854) = 42,212 + 174,246 = -132 \text{ J/mol/K} \dots$

3. $\Delta S_{\text{total}} = \Delta S_r + \Delta S_{\text{dispersed}} = 289,485 - 132 = +157,485 \text{ J/mol/K} \dots \text{J/K/mol} \dots$

4. $\Delta G_r = \Delta H_r - T \cdot \Delta S_r = -86,31 + 298,15 \cdot 0,132 = -46,9542 \dots \text{kJ/mol} \dots$
exoergic.....

$T \cdot \Delta S_{\text{total}} = +157,485 \text{ J/K/mol} \cdot 298,15 \text{ K} = +46,9542 \dots \text{kJ/mol} \dots$

bound $T\Delta S_{\text{total}} \leftarrow$ lost energy $\Delta G_{\text{reversereaction}} \leftarrow Q = +86,31 \text{ kJ/mol}$ **spontaneous** $\Delta G_{\text{reaction}} = -46,9542 \text{ kJ/mol} \dots$

THERMODYNAMICS Exercise XX Pyruvate $\text{H}_3\text{CC}=\text{O}\text{COO}^-$ decarboxylation $\text{H}_3\text{CCHO} + \text{HCO}_3^-$

Calculate ΔH_r , ΔS_r , ΔG_r at standard conditions 298.15 K. Reaction is **exothermic**, **athermic**, **endothermic**? Pyruvate $\text{H}_3\text{CC}=\text{O}\text{COO}^-$ conversion to acetaldehyde $\text{H}_3\text{CCHO} + \text{HCO}_3^-$ (25 C) 298.15 K, using the data table! Mention whether the reaction will be **exoergic** or **endoergic**!

Initial compounds Pyruvic acid+Q => products bicarbonate + H_3O^+

Substance	$\Delta H_r^\circ, \text{kJ/mol}$	$\Delta S_r^\circ, \text{J/mol/K}$
$\text{H}_3\text{CC}=\text{O}\text{COOH}_{(\text{aq})}$	-607,82	179,91
$\text{H}_3\text{CC}=\text{O}\text{COO}^-_{(\text{aq})}$	-603,7	-433,54
$\text{H}_3\text{CCHO}_{(\text{aq})}$	-212,23	160,2
H_3CCHO_l	-192,2	160,2
$\text{H}_2\text{O}_{(\text{aq})}$	-285,85	69,96
$\text{H}_3\text{O}^+_{(\text{aq})}$	-285,81	-3,854
HCO_3^-	-689,93	98,324



$$1. \Delta H_{\text{reaction}} = \sum \Delta H^\circ_{\text{products}} - \sum \Delta H^\circ_{\text{initial compounds}}$$

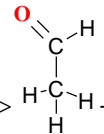
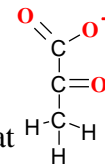
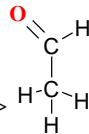
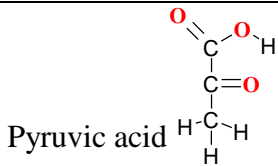
MassachusettsTinstitute

CRC

$$2. \Delta S_{\text{reaction}} = \sum \Delta S^\circ_{\text{products}} - \sum \Delta S^\circ_{\text{initial compounds}}$$

$$3. \Delta G_{\text{reaction}} = \Delta H_{\text{reaction}} - T \cdot \Delta S_{\text{reaction}}$$

$$3. \Delta G_{\text{reaction}} = \Delta H_{\text{reaction}} - T \cdot \Delta S_{\text{reaction}}$$



$$1. \Delta H_r = \Delta H^\circ_{\text{H}_3\text{CCHO}} + \Delta H^\circ_{\text{H}_3\text{O}^+} + \Delta H^\circ_{\text{HCO}_3^-} - 2 \Delta H^\circ_{\text{H}_2\text{O}} - \Delta H^\circ_{\text{H}_3\text{CC}=\text{O}\text{COOH}} = -8,45 \text{ kJ/mol} \dots \text{MassachusettsTinstitute}$$

$$\dots = -212,23 - 285,81 - 689,93 - (-2 \cdot 285,85 - 607,82) = -1187,97 + 1179,52 = -8,45 \text{ kJ/mol} \text{ exothermic} \dots$$

$$1. \Delta H_r = \Delta H^\circ_{\text{H}_3\text{CCHO}} + \Delta H^\circ_{\text{H}_3\text{O}^+} + \Delta H^\circ_{\text{HCO}_3^-} - 2 \Delta H^\circ_{\text{H}_2\text{O}} - \Delta H^\circ_{\text{H}_3\text{CC}=\text{O}\text{COO}^-} = +11,58 \text{ kJ/mol} \dots$$

$$\dots = -192,2 - 285,81 - 689,93 - (-2 \cdot 285,85 - 607,82) = -1187,97 + 1179,52 = 11,58 \text{ kJ/mol} \text{ endothermic} \dots$$

$$1. \Delta H_r = \Delta H^\circ_{\text{H}_3\text{CCHO}} + \Delta H^\circ_{\text{HCO}_3^-} - \Delta H^\circ_{\text{H}_2\text{O}} - \Delta H^\circ_{\text{H}_3\text{CC}=\text{O}\text{COO}^-} = +7,42 \text{ kJ/mol} \dots$$

$$\dots = -192,2 - 689,93 - (-285,85 - 603,7) = -882,13 + 889,55 = +7,42 \text{ kJ/mol} \text{ endothermic} \dots$$

$$2. \Delta S_{\text{dispersed}} = - \Delta H_r / T = 8,45 / 298,15 = +28,35 \text{ J/mol} \dots \text{MassachusettsTinstitute}$$

$$2. \Delta S_{\text{dispersed}} = - \Delta H_r / T = -11,58 / 298,15 = -38,8395 \text{ J/mol} \dots$$

$$2. \Delta S_{\text{dispersed}} = - \Delta H_r / T = -7,42 / 298,15 = -24,8868 \text{ J/mol} \dots$$

$$2. \Delta S_r = \Delta S^\circ_{\text{H}_3\text{CCHO}} + \Delta S^\circ_{\text{H}_3\text{O}^+} + \Delta S^\circ_{\text{HCO}_3^-} - 2 \Delta S^\circ_{\text{H}_2\text{O}} - \Delta S^\circ_{\text{H}_3\text{CC}=\text{O}\text{COOH}} = \dots \text{J/mol/K} \dots \text{MassachusettsTinstitute}$$

$$\dots = 160,2 - 3,854 + 98,324 - (2 \cdot 69,96 + 179,91) = -187,368 - 319,83 = -65,16 \text{ J/mol/K} \dots$$

$$2. \Delta S_r = \Delta S^\circ_{\text{H}_3\text{CCHO}} + \Delta S^\circ_{\text{H}_3\text{O}^+} + \Delta S^\circ_{\text{HCO}_3^-} - 2 \Delta S^\circ_{\text{H}_2\text{O}} - \Delta S^\circ_{\text{H}_3\text{CC}=\text{O}\text{COO}^-} = \dots \text{J/mol/K} \dots$$

$$\dots = 160,2 + 98,324 - (69,96 + 179,91) = 254,67 - 319,83 = -65,16 \text{ J/mol/K} \dots$$

$$2. \Delta S_r = \Delta S^\circ_{\text{H}_3\text{CCHO}} + \Delta S^\circ_{\text{HCO}_3^-} - \Delta S^\circ_{\text{H}_2\text{O}} - \Delta S^\circ_{\text{H}_3\text{CC}=\text{O}\text{COO}^-} = \dots \text{J/mol/K} \dots$$

$$\dots = 160,2 - 3,854 + 98,324 - (69,96 - 433,54) = 258,524 - 249,87 = 8,654 \text{ J/mol/K} \dots$$

$$3. \Delta S_{\text{total}} = \Delta S_r + \Delta S_{\text{dispersed}} = -65,16 - 28,35 = -36,81 \text{ J/mol/K} \dots \text{MassachusettsTinstitute}$$

$$3. \Delta S_{\text{total}} = \Delta S_r + \Delta S_{\text{dispersed}} = -65,16 - 38,8395 = -104 \text{ J/mol/K} \dots$$

$$3. \Delta S_{\text{total}} = \Delta S_r + \Delta S_{\text{dispersed}} = 8,654 - 24,8868 = -16,233 \text{ J/mol/K} \dots$$

$$4. \Delta G_r = \Delta H_r - T \cdot \Delta S_r = -8,45 - 298,15 \cdot (-0,06516) = +10,98 \text{ kJ/mol} \text{ endoergic} \dots \text{MassachusettsTinstitute}$$

$$4. \Delta G_r = \Delta H_r - T \cdot \Delta S_r = 11,58 - 298,15 \cdot (-0,06516) = +31,01 \text{ kJ/mol} \text{ endoergic} \dots$$

$$4. \Delta G_r = \Delta H_r - T \cdot \Delta S_r = 7,42 - 298,15 \cdot (-0,008654) = +4,84 \text{ kJ/mol} \text{ endoergic} \dots$$

$$T \cdot \Delta S_{\text{total}} = -36,81 \text{ J/mol} \cdot 298,15 \text{ K} = -10,97 \text{ kJ/mol} \dots \text{MassachusettsTinstitute}$$

$$\text{bound } T \Delta S_n \leftarrow \text{accumulate energy } \Delta G_{\text{reversereaction}} \leftarrow Q = -8,45 \text{ kJ/mol} \text{ not spontaneous } \Delta G_{\text{reaction}} = 10,98 \text{ kJ/mol} \dots$$

$$T \cdot \Delta S_{\text{total}} = -104 \text{ J/mol} \cdot 298,15 \text{ K} = -31,01 \text{ kJ/mol} \dots$$

$$\text{bound } T \Delta S_n \leftarrow \text{accumulate energy } \Delta G_{\text{reversereaction}} \leftarrow Q = 11,58 \text{ kJ/mol} \text{ not spontaneous } \Delta G_{\text{reaction}} = 31,01 \text{ kJ/mol} \dots$$

$$T \cdot \Delta S_{\text{total}} = -16,233 \text{ J/mol} \cdot 298,15 \text{ K} = -4,84 \text{ kJ/mol} \dots$$

$$\text{bound } T \Delta S_n \leftarrow \text{accumulate energy } \Delta G_{\text{reversereaction}} \leftarrow Q = 7,42 \text{ kJ/mol} \text{ not spontaneous } \Delta G_{\text{reaction}} = 4,84 \text{ kJ/mol} \dots$$

THERMODYNAMICS Exercise XXI Lactate $\text{H}_3\text{CCH}(\text{OH})\text{COO}^-_{\text{aq}}$ decarboxylation $\text{H}_3\text{CCH}_2\text{OH} + \text{HCO}_3^-$

Calculate ΔH_r , ΔS_r , ΔG_r at standard conditions 298.15 K. Reaction is **exothermic**, **athermic**, **endothermic**? Lactate $\text{H}_3\text{CC}=\text{OCOO}^-$ conversion to ethanol $\text{H}_3\text{CCHO} + \text{HCO}_3^-$ (25 C) 298.15 K, using the data table! Mention whether the reaction will be **exoergic** or **endoergic**! Initial compounds Lactate+Q => products ethanol bicarbonate

Substance	ΔH_r° , kJ/mol	ΔS_r° , J/mol/K
$\text{H}_3\text{CCH}(\text{OH})\text{COO}^-_{\text{aq}}$	-686,2	-557,71
$\text{H}_3\text{CCH}_2\text{OH}_1$	-277,6	160,7
$\text{H}_2\text{O}_{(\text{aq})}$	-285,85	69,96
HCO_3^-	-689,93	98,324

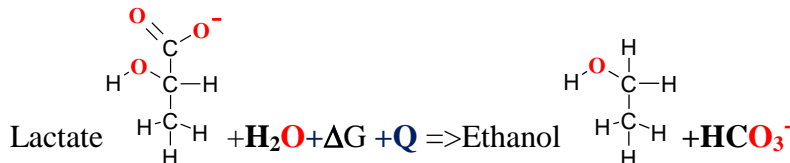


1. $\Delta H_{\text{reaction}} = \Sigma \Delta H^\circ_{\text{products}} - \Sigma \Delta H^\circ_{\text{initial compounds}}$

CRC

2. $\Delta S_{\text{reaction}} = \Sigma \Delta S^\circ_{\text{products}} - \Sigma \Delta S^\circ_{\text{initial compounds}}$

3. $\Delta G_{\text{reaction}} = \Delta H_{\text{reaction}} - T \cdot \Delta S_{\text{reaction}}$



1. $\Delta H_r = \Delta H^\circ_{\text{H}_3\text{CCH}_2\text{OH}} + \Delta H^\circ_{\text{HCO}_3^-} - \Delta H^\circ_{\text{H}_2\text{O}} - \Delta H^\circ_{\text{H}_3\text{CCH}_2\text{OHC(O)O}^-} = 4,52 \text{ kJ/mol} \dots \dots \dots$
 $\dots \dots \dots = -277,6 - 689,93 - (-285,85 - 686,2) = -967,53 + 972,06 = +4,52 \text{ kJ/mol}$ **endothermic**....

2. $\Delta S_{\text{dispersed}} = -\Delta H_r / T = -4,52 / 298,15 = -15,16 \dots \dots \dots \text{ J/K/mol} \dots$

2. $\Delta S_r = \Delta S^\circ_{\text{H}_3\text{CCH}_2\text{OH}} + \Delta S^\circ_{\text{HCO}_3^-} - \Delta S^\circ_{\text{H}_2\text{O}} - \Delta S^\circ_{\text{H}_3\text{CCH}_2\text{OHC(O)O}^-} = \dots \dots \dots \text{ J/mol/K} \dots$
 $\dots \dots \dots = 160,7 + 98,324 - (69,96 - 557,71) = 259,02 + 487,75 = 746,77 \text{ J/mol/K} \dots$

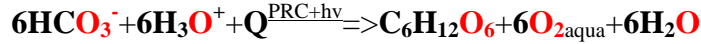
3. $\Delta S_{\text{total}} = \Delta S_r + \Delta S_{\text{dispersed}} = -15,16 + 746,77 = 731,61 \text{ J/mol/K} \dots \dots \dots \text{ J/mol/K}$

4. $\Delta G_r = \Delta H_r - T \cdot \Delta S_r = 4,52 - 298,15 \cdot 0,74677 = -218,13 \dots \dots \dots \text{ kJ/mol}$ **exoergic**.....

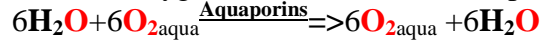
$T \cdot \Delta S_{\text{total}} = 731,61 \text{ J/K/mol} \cdot 298,15 \text{ K} = \mathbf{218,13} \dots \dots \dots \text{ kJ/mol} \dots$
 bound $T \Delta S_{\text{total}} \leftarrow$ accumulate energy $\Delta G_{\text{reversereaction}} \leftarrow Q = -4,52 \text{ kJ/mol}$ **spontaneous** $\Delta G_{\text{reaction}} = -218,13 \text{ kJ/mol} \dots$

THERMODYNAMICS Exercise XXII. Osmolar concentration gradient $11 = C_{osm}$ in green plants

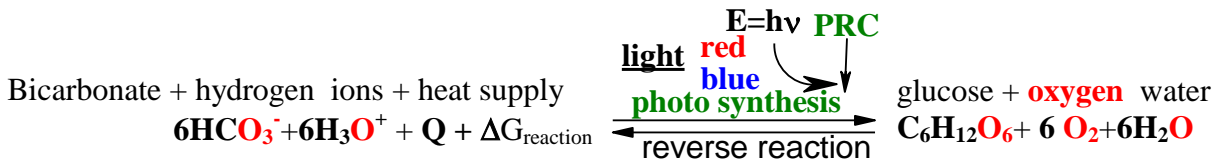
Calculate ΔH_r , ΔS_r , ΔG_r and the amount of heat **exothermic**, **athermic** or **endothermic** reaction at standard conditions 298.15 K. **PRC** Photo Synthetic Reaction Center ENZYME complex drive green plants products **C₆H₁₂O₆** and oxygen **6O₂_{aqua}**. by photon **E=h·v** absorption Aquaporin substrates oxygen **6O₂** and water **6H₂O** increase **osmotic** pressure to outside cell 11 times as concentration in cell decreases from initial times $12 = C_{osm} = 6 + 6$ to one glucose **C₆H₁₂O₆** molecule $C_{osm} = 1$. So total flow out of plant organisms through aquaporins increases 11 times:



against **osmolar** concentration gradient 12/1. Oxygen **6O₂** and water **6H₂O** pushed out



through Aquaporins in the **athermic** $\Delta H_{\text{channel}} = 0 \text{ kJ/mol}$ manners (as no heat waste) and used energy gained from **PRC** Photo Synthetic Reaction Center ENZYME complexes $\Delta G_{\text{PCR}} = 3040,1 \text{ kJ/mol}$ (Exercise III) via absorption red and blue Photon energy **E=h·v** and through heat supply **Q** p.3: <http://aris.gusc.lv/BioThermodynamics/BioChemicalProcesE.pdf>



Mention whether the reaction will be **exoergic** or **endoergic**! Universal gas constant $R = 8,3144 \text{ J/mol/K}$

$$\Delta G_{\text{channel}} = -RT \ln \left(\frac{C_{\text{osm}}[6\text{O}_{2\text{aqua}} + 6\text{H}_2\text{O}]_{\text{right}}}{C_{\text{osm}}[6\text{O}_{2\text{aqua}} + 6\text{H}_2\text{O}]_{\text{left}}} \right) = -12RT \ln(12/1) = -36.96 \text{ kJ/mol} \dots\dots\dots$$

Substance	before	after
O₂_{aqua}	$[\text{O}_2] = 6 \cdot 10^{-5} \text{ M}$	$[\text{O}_2] = 6 \cdot 10^{-5} \text{ M}$
H₂O	55,3 M	55,3 M

$$\Delta G_{\text{O}_2} = -RT \ln \left(\frac{[\text{O}_2]_{\text{right}}}{[\text{O}_2]_{\text{left}}} \right) = -RT \ln(K_{\text{equilibrium}}) = -6.1599 \dots\dots\dots$$

$$\dots\dots\dots = -8,3144 \cdot 298,15 \cdot \ln(12/1) = -8,3144 \cdot 298,15 \cdot -2.4849 = -6.1599 \text{ kJ/mol}$$

$$\text{For } 6\text{O}_{2\text{aqua}} \Delta G_{6\text{O}_2} = -6.1599 \cdot 6 = -36.9596 \dots\dots\dots \text{kJ/mol}$$

$$\Delta G_{6\text{H}_2\text{O}} = -6RT \ln \left(\frac{[\text{H}_2\text{O}]_{\text{right}}}{[\text{H}_2\text{O}]_{\text{left}}} \right) = 6 \cdot 8,3144 \cdot 310,15 \cdot \ln(1/12) = -36.9596 \dots\dots\dots \text{kJ/mol}$$

$$\text{For } 6\text{H}_2\text{O} \Delta G_{6\text{H}_2\text{O}} = -6.1599 \cdot 6 = -36.9596 \dots\dots\dots \text{kJ/mol}$$

.exoergic.....

.....

.....

.....

$$\Delta S_{6\text{O}_2} = -6R \ln \left(\frac{[\text{O}_2]_{\text{right}}}{[\text{O}_2]_{\text{left}}} \right) = -8,3144 \cdot \ln(1/12) = 20,66 \cdot 6 = 123.96 \dots\dots\dots \text{J/mol/K}$$

$$\Delta S_{6\text{H}_2\text{O}} = -6R \ln \left(\frac{[\text{H}_2\text{O}]_{\text{right}}}{[\text{H}_2\text{O}]_{\text{left}}} \right) = -8,3144 \cdot \ln(1/12) = 123.96 \dots\dots\dots \text{J/mol/K}$$

.....

.....

.....

$$\Delta H_{\text{channel}} = 0 \dots\dots\dots \text{kJ/mol} \dots\dots\dots \text{no heat waste} \dots\dots\dots$$

.....

$$T \cdot \Delta S_{6\text{O}_2} = -0,12396 \cdot 298,15 = 36.9596 \dots\dots\dots \text{kJ/mol used energy of PRC bound } T \Delta S_n = 3040,1 \text{ kJ/mol out off O}_2 \dots$$

$$T \cdot \Delta S_{6\text{H}_2\text{O}} = -0,12396 \cdot 298,15 = 36.9596 \dots\dots\dots \text{kJ/mol used energy of PRC bound } T \Delta S_n = 3040,1 \text{ kJ/mol out off H}_2\text{O}$$

.....

.....

.....

$$\text{For } 6\text{O}_{2\text{aqua}} + 6\text{H}_2\text{O} T \cdot \Delta S_{6\text{H}_2\text{O} + 6\text{O}_2} = 36.9596 + 36.9596 = 73.919 \dots\dots\dots \text{kJ/mol of PRC bound } T \Delta S_n = 3040,1 \text{ kJ/mol}$$

$$\text{athermic } \Delta H^\circ_{\text{reaction}} = +0 \text{ kJ/mol; } Q = -0 \text{ kJ/mol} \dots \text{spontaneous } \Delta G^\circ_{\text{reaction}} = -73.919 \text{ kJ/mol} \dots\dots\dots$$

The **Photosynthesis** dilutes of osmolar concentration by **6O₂_{aqua} + 6H₂O** consuming bicarbonate end hydrogen ions **6HCO₃⁻ + 6H₃O⁺** drive spontaneous flow of **6O₂_{aqua} + 6H₂O** through aquaporins out of **PRC** cells against membrane concentration gradient 12/1 with standard free energy $\Delta G_{6\text{H}_2\text{O} + 6\text{O}_2} = -73.919 \text{ kJ/mol}$ per one glucose mol **C₆H₁₂O₆**!