

Ūdeņraža elektroda atskaites punkta  $E^\circ_{\text{H}} = -0.2965$  Voltu atklāšana  
**absolūto potenciālu skalā** sinhronizē zinātnes ar **absolūtās** brīvās enerģijas skalu.

Mana šodienas runa ir vērsta uz pētījumiem par enerģijas un potenciālu **absolūto mērogu**, kas ir vienāds skaitlis ar pretēju zīmi apgrieztās reakcijas inversajā simetrijā.

Esmu patiesi priecīgs pievienoties jums 10. STARPTAUTISKAJĀ KONFERENCĒ par jaunām

Ķīmijas tendencēm vietnē ar atklājumu par tēmu:

Ūdeņraža elektroda atskaites punkta  $E^\circ_{\text{H}} = -0.2965$  Voltu atklāšana  
**absolūto potenciālu skalā** sinhronizē zinātnes ar **absolūtās** brīvās enerģijas skalu.

Ūdeņraža elektroda atskaites punkta  $E^\circ_{\text{H}} = -0.2965$  V atklāšana **absolūtā** potenciāla un **absolūtās** brīvās enerģijas skalai Nernsta pusreakcijā nosaka **inversās simetrijas** īpašību: Apgrieztais reakcijas potenciāls pieder vienam un tam pašam skaitlim ar pretēju zīmi.

Simetrija sakrīt ar **inverso absolūto** brīvo enerģiju, kuras skaitlis ir vienāds, bet ar pretēju zīmi.

**Absolūtās** un **inversās** brīvās enerģijas un potenciāla mēroga noteikšanai nepieciešama ūdens un hidroksionija uzskaitē, kuras pamatā ir Alberty dati par ūdeņraža gāzi un šķīduma absolūtās brīvās enerģijas vērtību.

Nernsta klasiskā pusreakcija ar ūdens un hidroksionija atlaidi ir  $\underline{\text{H}}(\text{Pt}) = \text{H}^+ + \text{e}^-$ . [11]

Standarta klasiskais potenciāls nulle  $E^\circ_{\text{H}} = 0.0$  V tiek ņemts  $[\text{H}^+] = 1$  M sērskābes šķīdumā nomērīts potenciāls:

$$E = E^\circ_{\text{H}} + 0.0591 \cdot \log[\text{H}^+] = 0.0 + 0.0591 \cdot \log(1 \text{ M}) = 0 \text{ V}$$

un ir nulls atskaitē klasiskā potenciālu skalā kopš 1920. gada Nobela prēmijas ķīmijā

Termodinamiskā pusreakcija ar ūdens un hidroksionija uzskaiti ir  $\underline{\text{H}}(\text{Pt}) + \text{H}_2\text{O} = \text{H}_3\text{O}^+ + \text{e}^-$ .

Termodinamiskā potenciāla izteiksme pusreakcijai uz ņemtā nulles potenciāla  $E = 0$  V vērtības ir:

$$E = E^\circ_{\text{H}} + 0.0591 \cdot \log\left(\frac{[\text{H}_3\text{O}^+]}{[\text{H}_2\text{O}]}\right) = 0.10166 + 0.0591 \cdot \log(1 \text{ M}/52.5 \text{ M}) = 0 \text{ V}$$

kur  $0.0591 \cdot \log(1/52.5) = -0.10166$  V ir termodinamiskā standarta potenciāla korekcija.

Ūdens uzskaitē koriģē termodinamisko standarta potenciālu:  $E^\circ_{\text{H}} = 0.10166$  V termodinamiskā potenciāla skalā

nulles vietā:  $E = E^\circ_{\text{H}} + \frac{\ln(10) \cdot R \cdot T}{F \cdot 1 \text{e}^-} \cdot \log\left(\frac{[\text{H}_3\text{O}^+]}{[\text{H}_2\text{O}]}\right) = 0 \text{ V}$ ;  $E^\circ_{\text{H}} = E - 0.0591 \cdot \log(1/52.5) = 0 - (-0.10166) = 0.10166 \text{ V}$ .

Attiecība  $[\text{H}_3\text{O}^+]/[\text{H}_2\text{O}] = 1/52.5$  dod koriģēto termodinamisko standarta potenciālu  $E^\circ_{\text{H}} = 0.10166$  V nulles vietā.

Nernsta pusreakcijā ūdeņradim  $\underline{\text{H}}(\text{Pt}) + \text{H}_2\text{O} = \text{H}_3\text{O}^+ + \text{e}^-$  standarta punkta absolūtais potenciāls ir

$$E^\circ_{\text{H}} = -0.29654 \text{ V}.$$

Nernsta pusreakcija **absolūtajā** standarta **potenciāla** producētā izmaiņas vērtība brīvās enerģijas skalā:

$$\Delta G_{\text{eq}} = E^\circ_{\text{H}} \cdot F \cdot 1 = -0.29654 \cdot 96485 \cdot 1 = -28.61 \text{ kJ/mol}$$

ir identisks Hesa likumā aprēķinātās brīvās enerģijas izmaiņai kā eksoergiskai absolūtajā skalā, kas attiecas uz ūdens nulles brīvās enerģijas saturu  $G_{\text{H}_2\text{O}} = 0 \text{ kJ/mol}$ :

$$\Delta G_{\text{Hess}_{\text{eq}}} = G_{\text{H}_3\text{O}^+} + G_{\text{e}^-} - (G_{\text{H}(\text{Pt})} + G_{\text{H}_2\text{O}}) = 22.44 + 0 - (51.05 + 0) = -28.61 \text{ kJ/mol}.$$

**Absolūtais** standarta **potenciāls**  $E^\circ_{\text{H}} = -0.29654$  Volti sakrīt ar Alberty datu **absolūtās** brīvās enerģijas skalu.

[8,15]

**Absolūtā OxRed potenciālu skala noslīd par  $\Delta E = -0,29654 - 0,10166 = -0,3982$  Voltiem zemāk. Ūdens uzskaitē zinātnēs pieprasa absolūto brīvās enerģijas skalu sinhronizējot Nernsta reakciju absolūto potenciālu skalu inversās simetrijas identiskās vērtībās bet ar pretēju zīmi.**

Atraktoram  $pH=7,36$  līdzsvara stāvoklī ir patiesa  $pOH=6,64$  vērtība, jo  $pK_w=14 = pH+pOH = 7,36 + 6,64$ .

Ūdens daudzuma atlaide  $[H_2O]=963/18=53,5$  M litrā sērskābes  $[H_2SO_4]=[H_3O^+]=1$  M šķīduma ar  $1,061$  g/mL blīvumu **ūdeņraža elektrodam** Nernsta izteiksmē ir klasiska standarta potenciāla  $E_{o\_classic}=0$  V atskaites vērtība:

$$\underline{H(Pt)}=H^++e^-; E_{classic}=E_{o\_classic}+0,0591 \cdot \log K^o_{classicH(Pt)}=0+0,0591 \cdot \log[H^+]=0+0,0591 \cdot \log(1 \text{ M})=0 \text{ Volti. [11]}$$

Termodinamiska hidroksionija jonu uzskaitē pieprasa ūdeni:  $\underline{H(Pt)}+H_2O \rightleftharpoons H_3O^++e^-$  un  $E^o_H=0,10166$  V.

Attiecība  $[H_3O^+]/[H_2O]=1 \text{ M}/52,5 \text{ M}=X_{H_3O^+}/X_{H_2O}$  ir mol daļa aizstājot molaritāti  $[H^+]=1$  M klasiskajā potenciāla izteiksmē. Ūdens uzskaitē dod termodinamisko standartu  $E^o_H=0,10166$  V potenciālu skalā.

Nernsta izteiksme ar klasisko mērījumu nulle pieprasa termodinamisko standarta potenciālu  $E^o_H=0,10166$  V :

$$E=E^o_H+\frac{\ln(10) \cdot R \cdot T}{F \cdot 1} \cdot \log \frac{X_{H_3O^+}}{X_{H_2O}} =E_o+E^o_H+0,0591 \cdot \log(1/52,5)=0,10166-0,10166=0 \text{ V.}$$

Ja attiecība ir viens  $1=K_{H(Pt)}=X_{H_3O^+}/X_{H_2O}$ , tad potenciāls  $E^o_H=0,10166$  V ir termodinamiskais standarts:

$$E=E^o_H+\frac{\ln(10) \cdot R \cdot T}{F \cdot 1} \cdot \log \frac{X_{H_3O^+}}{X_{H_2O}} =0,10166+0,0591 \cdot \log(1)=0,10166 \text{ V.}$$

Metāla oksidēšanas brīvās enerģijas izmaiņa ir atšķirīga endoerģiska  $\Delta G_{eq}=E^o_H \cdot F \cdot 1=0,10166 \cdot 96485 \cdot 1=9,81$  kJ/mol pretstatā Alberty eksoerģiskai.

**Alberty** Hesa vērtība ir eksoerģiska:  $\Delta G_{Hess\_eq}=G_{H_3O^+}+G_{e^-}-(G_{H(Pt)}+G_{H_2O})=22,44+0-(51,05+0)=-28,61$  kJ/mol .

Brīvās enerģijas izmaiņa ir noteikta nulles atskaites skalā  $G_{H_2O}=G_{CO_2\text{gas}}=G_{e^-}=0$  kJ/mol. Iteratīvi izskaitļotais absolūtajā skalā ūdeņraža standarta potenciāls ir:  $E^o_H=-0,29654$  Volti. Līdzsvara brīvās enerģijas minimums ir eksoerģisks:  $\Delta G_{eq}=E^o_H \cdot F \cdot 1=-0,29654 \cdot 96485 \cdot 1=-28,61$  kJ/mol sakrīt ar Alberty datiem. Absolūtā potenciālu skala noslīd par  $\Delta E=-0,29654-0,10166=-0,3982$  Voltiem zemāk. Nernsta līdzsvara konstante ir lielāka par vienu:

$$K_{H(Pt)\_Red}=[H_3O^+][e^-]/[H_2O]/[H(Pt)]=EXP(-\Delta G_{Alberty}/R/T)=EXP(28612/8,3144/298,15)=102954 .$$

I veida elektrodos metāls  $\underline{H(Pt)}$  / iegremdēts tā katjonu  $H_3O^+$  šķīdumā pielietojums.

Liela ātruma protolīzes atraktori  $[H_3O^+]=10^{-7,36}$  M ,  $pH=7,36$  un ūdens masas  $[H_2O]=997/18=55,3$  M uzskaitē litrā rāda metāla ūdeņraža stipru reducējošu potenciālu:  $E_{pH=7,36}=-0,29654+0,0591 \cdot \log(10^{-7,36}/55,3)=-0,8345$  V un brīvās enerģijas izmaiņas minimumu  $\Delta G_{eqpH=7,36}=E^o_H \cdot F \cdot 1=-0,8345 \cdot 96485 \cdot 1/1000=-80,5$  kJ/mol .

Nernsta pus reakcijas metāla reducēšanas līdzsvara potenciāla  $E^o_H=-0,29654$  V enerģija ir  $\Delta G_{eq}=-28,6$  kJ/mol.

Platīna plāksnīte iemērta hidroksionija jonu  $[H^+]=[H_3O^+]=[H_2SO_4]=1$  M sērskābes

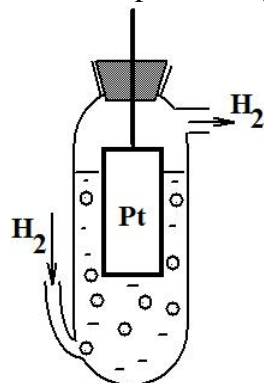
šķīdumā  $\underline{H(Pt)}=H^++e^-$ :  $E=E^o+0,0591 \cdot \log[H^+]=0,0+0,0591 \cdot \log(1 \text{ M})=0$  V ir klasika.

Attiecība  $[H_3O^+]/[H_2O]=1/52,5=X_{H_3O^+}/X_{H_2O}$  dod klasiskās nulles **0** vietā termodinamisko standarta potenciālu:  $E^o_H=0,10166$  V . Absolūtais standarta potenciāls  $E^o_H=-0,29654$  V

pamatojas uz Alberty ūdeņraža datiem  $G_{H_2\text{gas}}=85,64$  kJ/mol un  $G_{H_2\text{aq}}=103,24$  kJ/mol , kuri ir noteikti ūdens un oglekļa dioksīda gāzes nulles atskaites skalā  $G_{H_2O}=G_{CO_2\text{gas}}=0$  kJ/mol.

absolūti $E^o_H=-0,29654$ V	klasiska nulle $E^o_H=0$ V	$0,10166$ V	$E, V$
$E_{(Pt)H/H^+}=E^o_H+0,0591 \cdot \log\left(\frac{X_{H_3O^+}}{X_{H_2O}}\right)$			
$E_{H\_classic}=E^o_H+0,0591 \cdot \log([H_3O^+])$			
$E^o_H$ termodinamiskais			

Pie  $pH=7,36$  ,  $[H_3O^+]=10^{-7,36}$  M ar potenciālu  $E=-0,2965+0,0591 \cdot \log(10^{(-7,36)}/55,3)=-0,8345$  V metāls  $\underline{H(Pt)}$  ir stiprs reducētājs. Brīvās enerģijas saturs vienā molā ūdeņraža metāla ir:  $G_{H(Pt)}=51,05$  kJ/mol.



Inversā pus reakcijā producējas ūdens  $O_{2\text{aqua}} + 2H_{2\text{aqua}} \Rightarrow 2H_2O$ . Hesa brīvās enerģijas izmaiņa ir eksoerģiska:  $\Delta G_{\text{eq}2H_2O} = 6G_{H_2O} - (G_{O_{2\text{aqua}}} + 4G_{H_3O^+}) = 6 \cdot 0 - (330 + 4 \cdot 22.44) = -419.76 \text{ kJ/mol}$  **inversā absolūtā** standarta potenciālā -  $E^\circ_{O_2} = -1.0868 \text{ V}$ . Brīvās enerģijas izmaiņa ir negatīva  $\Delta G_{\text{eq}} = -E^\circ_{O_2} \cdot F \cdot 1 \cdot 4 = -1.0868 \cdot 96485 \cdot 4 = -419.44 \text{ kJ/mol}$  un sakrīt ar Alberty datiem eksoerģisku Hesa vērtību pus reakcijai.

Četras reducējošas pus reakcijas  $4H(\text{Pt}) + 4H_2O = 4H_3O^+ + 4e^-$ ,  $E^\circ_H = -0.2965 \text{ V}$  dod brīvās enerģijas izmaiņas minimum  $\Delta G_{\text{eq}} = (E^\circ_H - E^\circ_{O_2}) \cdot F \cdot 4 = (-0.2965 - 1.0868) \cdot 96485 \cdot 4 = -1.38334 \cdot 96485 \cdot 4 / 1000 = -533.9 = 2 \cdot -266.94 \text{ kJ/mol}$  ūdeni producējot  $O_{2\text{aqua}} + 4H(\text{Pt}) = 2H_2O$  no elementiem ar enerģijas saturu  $G_{H(\text{Pt})} = 51 \text{ kJ/mol}$  un  $G_{O_{2\text{aq}}} = 330 \text{ kJ/mol}$ .

Ūdeņraža oksidēšanas reakcijā par ūdeni  $O_{2\text{aqua}} + 2H_{2\text{aqua}} \Rightarrow 2H_2O$  Hesa **absolūtās** brīvās enerģijas izmaiņa arī tik pat eksoerģiska:  $\Delta G_{\text{Hess}H_2O\text{aqua}} = (2G_{H_2O} - (2G_{H_{2\text{aqua}}} + G_{O_{2\text{aqua}}})) / 2 = (0 - (2 \cdot 103 + 330)) / 2 = -268 \text{ kJ/mol}$  sakrīt ar **absolūto** potenciāla enerģijas skalu  $\Delta E_{\text{eq}H_2O} = (E^\circ_H - E^\circ_{O_2}) / 2 = (-0.2965 - 1.0868) / 2$  enerģijai  $\Delta G_{\text{eq}H_2O} = -266.94 \text{ kJ/mol}$ .

Hesa vienādojumā  $\Delta G_{\text{eq}2H_2O} = 2G_{H_2O} - 4G_{H(\text{Pt})} - G_{O_{2\text{aqua}}} = 2 \cdot 0 - (4 \cdot 51 + 330) = -533.9 = 2 \cdot -267 \text{ kJ/mol}$  iegūstams metāla **absolūtās** brīvās enerģijas saturs  $G_{H(\text{Pt})} = (2G_{H_2O} - \Delta G_{\text{eq}2H_2O} - G_{O_{2\text{aqua}}}) / 4 = (2 \cdot 0 + 533.886 - 330) / 4 = 51.05 \text{ kJ/mol}$ . **Absolūtās** brīvās enerģijas saturs ir aprēķināts ūdens un gāzes  $CO_{2\text{gas}}$  nulles skalā  $G_{H_2O} = G_{CO_{2\text{gas}}} = 0 \text{ kJ/mol}$ .

Ūdeņraža metāls ir iekļauts platīna režģī ar  $G_{H(\text{Pt})} = 51 \text{ kJ/mol}$ , elements slāpekļis satur  $G_{N_{2\text{gas}}} = -15.26 \text{ kJ/mol}$ , skābekļa gāze  $G_{O_{2\text{gas}}} = 303 \text{ kJ/mol}$  plus  $G_{O_{2\text{sp}}} = 26.58 \text{ kJ/mol}$  šķīdība ūdenī veido  $G_{O_{2\text{aqua}}} = 330 \text{ kJ/mol}$ ,

for graphite in reaction with oxygen gas and hydrogen gas  $G_{\text{graphite}} = G_{CO_{2\text{gr}}} = G_{C_{\text{gr}}CH_{4\text{gas}}} = 91.26 \text{ kJ/mol}$ .

Šķīdības  $O_{2\text{gas AIR}} + H_2O \xrightarrow{\text{Aquaporins}} O_{2\text{aq}}$  konstantes enerģija palielinās par  $G_{O_{2\text{sp}}} = 26.58 \text{ kJ/mol}$ :

$$[O_{2\text{aq}}] / [O_{2\text{gas Gauss}}] / [H_2O] = K_{\text{šķ}} = 2.205 \cdot 10^{-5}. G_{O_{2\text{šķ}}} = -R \cdot T \cdot \ln(K_{\text{šķ}}) = -8.3144 \cdot 298.15 \cdot \ln(2.205 \cdot 10^{-5}) = 26.58 \text{ kJ/mol}.$$

Dati no [CRC](#) gāzēm  $O_{2\text{gas}} + 2H_{2\text{gas}} \Rightarrow 2H_2O$  uz vienu mola saturu ūdenim ir  $\Delta G_{\text{Hess}H_2O} = -237.19 \text{ kJ/mol}$ .

Skābekļa viens mols satur  $G_{O_{2\text{gas}}} = 2 \cdot G_{H_2O} - 2 \cdot (\Delta G_{\text{Hess}H_2O} + G_{H_{2\text{gas}}}) = 2 \cdot 0 - 2 \cdot (-237.19 + 85.64) = 303 \text{ kJ/mol}$  reakcijā no elementiem  $\Delta G_{\text{Hess}H_2O\text{BioChem}} = (2G_{H_2O} - (2G_{H_{2\text{gas}}} + G_{O_{2\text{gas}}})) / 2 = (0 - (2 \cdot 85.64 + 303)) / 2 = -237.19 \text{ kJ/mol}$ . [1,8]

$$\text{CRC [1]} \Delta G_{\text{Hess}H_2O} = -237.19 \text{ kJ/mol} = (2G_{H_2O} - (2G_{H_{2\text{gas}}} + G_{O_{2\text{gas}}})) / 2 = -237.19 \text{ kJ/mol} = \Delta G_{\text{Hess}H_2O\text{BioChem}}. \text{ Alberty [8]}$$

Dati no [1] un [8] ir sakrītoši  $-237.19 \text{ kJ/mol} = -237.19 \text{ kJ/mol}$ . **Absolūtā** enerģija ūdens šķīdumos arī ir  $G_{H_{2\text{aqua}}} = 103 \text{ kJ/mol}$  and  $G_{O_{2\text{aqua}}} = G_{O_{2\text{gas}}} + G_{O_{2\text{šķ}}} = 303 + 26.58 = 330 \text{ kJ/mol}$  eksoerģiska  $O_{2\text{aqua}} + 2H_{2\text{aqua}} = 2H_2O$ :

$$G_{\text{Hess}H_2O\text{BioChem}} = (2G_{H_2O} - (2G_{H_{2\text{aqua}}} + G_{O_{2\text{aqua}}})) / 2 = (2 \cdot 0 - (2 \cdot 103 + 330)) / 2 = -268 \text{ kJ/mol}.$$

[Alberty](#) dati ūdeņraža gāzei  $G_{H_{2\text{gas}}} = 85.64 \text{ kJ/mol}$  un ūdeņraža šķīdumam  $G_{H_{2\text{aqua}}} = 103 \text{ kJ/mol}$  tiek lietoti šķīdības konstantes reakcijai ūdenī:  $H_{2\text{gas}} + H_2O \rightleftharpoons H_{2\text{aq}}$ . Ūdeņraža šķīdības destilētā ūdenī **absolūta** enerģijas izmaiņa ir:

$$\Delta G_{H_{2\text{šķ}}\text{Alberty}} = G_{H_{2\text{aq}}} - G_{H_{2\text{gas}}} - G_{H_2O} = 103.24 - 85.64 - 0 = 17.6 \text{ kJ/mol}.$$

[Alberty](#) bioķīmijas matemātiskā pielietojuma dati veido šķīdības konstanti mol daļās  $K_{H_{2\text{šķ}}} = 0.0008253$ :

$$[H_{2\text{aq}}] / [H_{2\text{gas}}] / [H_2O] = K_{H_{2\text{šķ}}} = \text{EXP}(-\Delta G_{H_{2\text{šķ}}\text{Alberty}} / R / T) = \text{EXP}(-17600 / 8.3144 / 298.15) = 0.0008253 \text{ ar šķīdību}$$

$$[H_{2\text{aq}}] = K_{H_{2\text{šķ}}} \cdot [H_2O] = 0.0008253 \cdot 55.3 = 0.04564 \text{ M, ja tīras gāzes mol daļa ir viens } [H_{2\text{gas}}] = 1. [8]$$

$H_{2\text{gas}} + H_2O \Rightarrow H_{2\text{aqCRC}}$ ; Šķīdība 100 gramos destilēta ūdens  $0.000155 \text{ g/100g}_{H_2O}$ , blīvums  $0.996 \text{ g/L}$  veido koncentrāciju  $[H_{2\text{aqCRC}}] = 0.000155 / 2 / 100.000155 \cdot 996 = 0.0007719 \text{ M}$ , [1] CRC

Šķīdības konstante  $K_{\text{šķCRC}} = [H_{2\text{aq}}] / [H_2O] = 0.0007719 / 55.3 = 0.000013958$  un **absolūtā** brīvās enerģijas izmaiņa ir  $\Delta G_{\text{šķ}H_2\text{CRC}} = -R \cdot T \cdot \ln(K_{\text{šķ}H_2\text{CRC}}) = -8.3144 \cdot 298.15 \cdot \ln(0.000013958) = 27.7 \text{ kJ/mol}$ .

Bioķīmiskā ūdenī eksoerģiska šķīdība  $G_{H_{2\text{šķ}}\text{Alberty}} = G_{H_{2\text{aq}}} - G_{H_{2\text{gas}}} - \Delta G_{H_2O\text{Biochemistry}} = 103.24 - 85.64 - 85.6 = -68 \text{ kJ/mol}$ :

$$[H_{2\text{aq}}] / [H_{2\text{gas}}] / [H_2O] = K_{H_{2\text{šķ}}\text{Biochemistry}} = \text{EXP}(-\Delta G_{H_{2\text{šķ}}\text{Alberty}} / R / T) = \text{EXP}(68000 / 8.3144 / 298.15) = 10^{11.9} \text{ ar}$$

koncentrāciju  $[H_{2\text{aq}}] = K_{H_{2\text{šķ}}\text{Biochemistry}} \cdot [H_2O] = 10^{11.9} \cdot 55.3 = 10^{13.6} \text{ M}$ , ja tīras ūdeņraža  $H_{2\text{gas}}$  gāzes mol daļa ir viens  $[H_{2\text{gas}}] = 1$ . [8]

Nernsta  $\text{H}_{2\text{aq}}+2\text{H}_2\text{O}=\text{H}_3\text{O}^++2\text{e}^-$  ūdeņraža oksidēšana par hidroksioniju ie patvaļīga, jo **absolūtā** brīvā enerģija ir pozitīva.  $\Delta G_{\text{Hess, H}_3\text{O}^+}=\text{G}_{\text{H}_2\text{aq}}+2\text{G}_{\text{H}_2\text{O}}-(2\text{G}_{\text{H}_3\text{O}^+}+2\text{G}_{\text{e}^-})=2*22.44+2*0-(103.24+2*0)=-58.36 \text{ kJ/mol}$ .

Ar grafitu oksidē  $\text{H}_{2\text{aq}}$  šķīdumu par hidroksioniju ar **absolūto** standarta potenciālu:

$$E^\circ_{\text{H}_3\text{O}^+}=-58.36*1000/96485/2=-0.302 \text{ V}.$$

$\text{H(Pt)}$  pus reakcijas **inversais** standarta potenciāls  $-E^\circ_{\text{H(Pt)}}=+0.2965 \text{ V}$  un Nernsta ūdeņraža šķīduma oksidēšanas pus reakcija sumā  $E^\circ_{\text{H}_3\text{O}^+}=-0.302 \text{ V}$   $\text{H}_{2\text{aq}}+2\text{H}_2\text{O}=\text{H}_3\text{O}^++2\text{e}^-$ ;  $2\text{H}_3\text{O}^++2\text{e}^-=\text{H(Pt)}+2\text{H}_2\text{O}$ ;  $-E^\circ_{\text{H(Pt)}}=+0.2965 \text{ V}$  uzrāda ūdeņraža mol daļas  $[\text{H}_{2\text{aqAlberty}}]$  šķīdību metālā eksoerģiski patvaļīgu:

$$\text{H}_{2\text{aqAlberty}}=2\text{H(Pt)}; \text{K}_{\text{Alberty, šķH(Pt)}}=[\text{H(Pt)}]^2/[\text{H}_{2\text{aqAlberty}}] \text{ mol daļu koncentrācijās bez mērvienībām:}$$

$$\Delta G_{\text{elektro, šķH(Pt)}}=\Delta E^\circ_{\text{šķH(Pt)}}*F*2=(E^\circ_{\text{H}_3\text{O}^+}-E^\circ_{\text{H(Pt)}})*F*2=(-0.302+0.2965)*96485*2=-0.0055*96485*2=-1.06 \text{ kJ/mol};$$

$$\text{K}_{\text{Alberty, šķH(Pt)}}=[\text{H(Pt)}]^2/[\text{H}_{2\text{aqAlberty}}]=\text{EXP}(-\Delta G_{\text{Alberty}}/R/T)=\text{EXP}(1060/8.3144/298.15)=1,5336 . [8]$$

Šķīdības konstante reakcijā  $\text{H}_{2\text{aqAlberty}}=2\text{H(Pt)}+\text{H}_2\text{O}$ ;  $\text{K}_{\text{Alberty, šķH(Pt)}}=[\text{H(Pt)}]^2*[\text{H}_2\text{O}]/[\text{H}_{2\text{aqAlberty}}]$  uzrāda ūdeņraža mol daļas bez mērvienībām  $[\text{H}_{2\text{aqAlberty}}]/[\text{H}_2\text{O}]$  šķīdības konstanti metālā eksoerģisku:

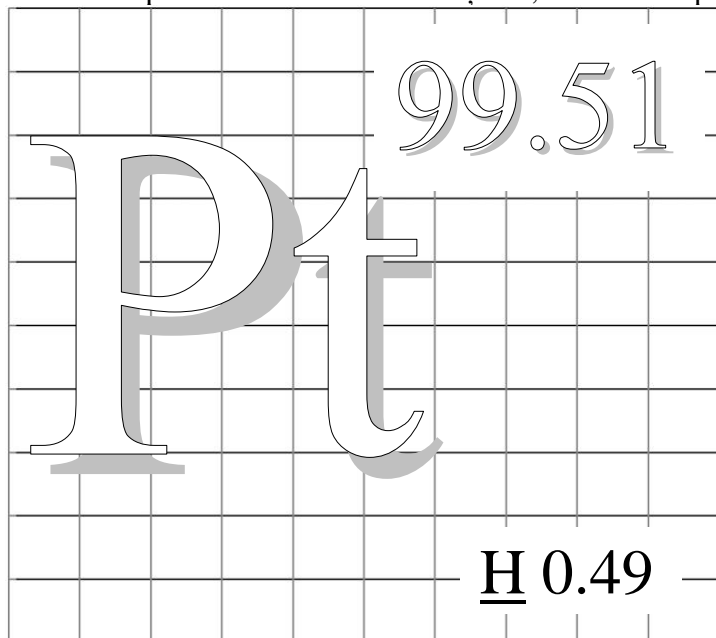
$$\Delta G_{\text{Alberty, šķH(Pt)}}=2\text{G}_{\text{H(Pt)}}+\text{G}_{\text{H}_2\text{O}}-(\text{G}_{\text{H}_{2\text{aq}}})=2*51.05+0-(103.24)=-1.14 \text{ kJ/mol} .$$

$$\text{K}_{\text{Alberty, šķH(Pt)}}=[\text{H(Pt)}]^2*[\text{H}_2\text{O}]/[\text{H}_{2\text{aqAlberty}}]=\text{EXP}(-\Delta G_{\text{Alberty}}/R/T)=\text{EXP}(1140/8.3144/298.15)=1,584 . [8]$$

$[\text{H(Pt)}]^2/[\text{H}_{2\text{aqAlberty}}]=\text{K}_{\text{Alberty, šķH(Pt)}}/[\text{H}_2\text{O}]=1,58387/55.3=0,02864 \text{ M}$  ja  $[\text{H}_{2\text{aqAlberty}}]=0.0008253 \text{ mol}$  daļa ir piesātinājumā. Mol daļas šķīdības kvadrāta laukums ir:

$$[\text{H(Pt)}]^2=\text{K}_{\text{šķH(Pt)}}/[\text{H}_2\text{O}]*[\text{H}_{2\text{aqAlberty}}]=1.584/55.3*0,0008253=0,00002364.$$

Mol daļas šķīdība  $[\text{H(Pt)}]=\text{SQRT}(1,584/55,3*0,0008253)=0,004862$  ir ūdeņraža atomu virsmas daļa 0,486% dalties ar platīna atomu virsmas daļu 99,514% no kopējā 100% platīna kristāla virsmas.



Piesātināta ūdeņraža  $\text{H(Pt)}$  metāla mol daļa ir:

$$[\text{H(Pt)}]=\text{SQRT}(0,00002364)=0,004862=0,49 \text{ mazāka par vienu, ja tīras gāzes mol daļa ir viens } [\text{H}_{2\text{gas}}]=1.$$

Mol daļa šķīdības ir ūdeņraža virsmas daļa procentos 0,49%, ar kuru dalās platīna atomu daļa 99,51% uz kopējās platīna kristāla virsmas 100% laukuma. Viens kvadrāts  $1\text{ m}^2$  ir viens percents 1% no virsmas un 100 kvadrāti ir 100%, jo  $10*10=100\text{ m}^2$ . Šķīdības  $\text{H}_{2\text{aqAlberty}}=2\text{H(Pt)}+\text{H}_2\text{O}$  koncentrāciju mol daļas ir bez mērvienībām kā konstante arī:  $\text{K}_{\text{Alberty, šķH(Pt)}}=1,584$ .

Atomu radiusi ir Pt 0.135 nm and H 0,053 nm.

Atomu kvadrātu laukumi uz virsmas ir Pt  $0.0729 \text{ nm}^2$  un H  $0.0112 \text{ nm}^2$ . Divi atomi  $0.0729+0.0112=0.0841 \text{ nm}^2$  dalās virsmas kopējā laukumā 100% . Platīna atomam ir  $0.0729/0.0841=86.7\%$  un  $0.0112/0.0841=9,53\%$  pieder ūdeņraža atomam. [25]

$\text{H(Pt)}$  šķīdība ūdenī ir mazāka par vienu  $\text{K}_{\text{šķH(Pt)}}=0.631$ :

$$2\text{H(Pt)}+\text{H}_2\text{O}=\text{H}_{2\text{aqAlberty}}; \text{K}_{\text{šķH(Pt)}}=[\text{H(Pt)}]^2*[\text{H}_2\text{O}]/[\text{H}_{2\text{aq}}];$$

$$\Delta G_{\text{Alberty}}=\text{G}_{\text{H}_{2\text{aq}}}+2\text{G}_{\text{H(Pt)}}-\text{G}_{\text{H}_2\text{O}}=1.14 \text{ kJ/mol};$$

$$\text{K}_{\text{šķH(Pt)}}=[\text{H}_{2\text{aq}}]/[\text{H(Pt)}]^2/[\text{H}_2\text{O}]=\text{EXP}(-\Delta G_{\text{šķH(Pt)}}/R/T)=\text{EXP}(-1140/8.3144/298.15)=0.631 \text{ unfavored. [8]}$$

Ūdens oksidēšana par skābekli pus reakcijas  $5\text{H}_2\text{O}=\text{O}_{2\text{aq}}+4\text{H}_3\text{O}^++4\text{e}^-$  Hesa brīvās enerģijas izmaiņa ir:

$$\Delta G_{\text{O}_{2\text{aqAlberty}}}=\text{G}_{\text{O}_{2\text{aq}}}+4\text{G}_{\text{H}_3\text{O}^+}-5\text{G}_{\text{H}_2\text{O}}=330-4*22,44-5*0=419,76 \text{ kJ/mol} , \text{ jo aqua moldaļa}$$

$\text{O}_{2\text{gas AIR}}+\text{H}_2\text{O}=\text{O}_{2\text{aq}}$  kompensē sesto ūdens molekulu  $6\text{H}_2\text{O}=\text{O}_{2\text{gas AIR}}+\text{H}_2\text{O}+4\text{H}_3\text{O}^++4\text{e}^-$  un Nernsta pusreakcija ir:  $5\text{H}_2\text{O}=\text{O}_{2\text{aq}}+4\text{H}_3\text{O}^++4\text{e}^-$  ar absolūto standarta potenciālu  $E^\circ_{\text{O}_{2\text{aq}}}=1,0610 \text{ V}$ .

Tā ir identiska brīvās enerģijas izmaiņas minimumam elektroķīmiskos aprēķinos lietojot absolūto Nernsta standarta potenciālu  $E^\circ_{\text{O}_{2\text{aq}}}=1,0610 \text{ Volti}$ :  $\Delta G_{\text{eqO}_{2\text{aq}}}=\text{E}^\circ_{\text{O}_{2\text{aq}}}\cdot F\cdot n_{\text{e}^-}=1,0610*96485*4=409,5 \text{ kJ/mol} .$

Metāla ūdeņraža  $\text{H(Pt)}$  pus reakcijas  $\text{H(Pt)}+\text{H}_2\text{O}=\text{H}_3\text{O}^++\text{e}^-$  Hesa brīvās enerģijas izmaiņa ir:

$$\Delta G_{\text{H(Pt)eqAlberty}}=\text{G}_{\text{H}_3\text{O}^+}+\text{G}_{\text{e}^-}-(\text{G}_{\text{H}_2\text{O}}+\text{G}_{\text{H(Pt)}})=22,44+0-(0+51,05)=-28,61 \text{ kJ/mol} .$$

Tā ir identiska elektroķīmiskiem brīvās enerģijas izmaiņas minimuma aprēķiniem lietojot **absolūto** Nernsta standarta potenciālu  $E^\circ_{\text{H(Pt)}}=-0,29654 \text{ Volti}$  :

$$\Delta G_{\text{eqH(Pt)}}=\text{E}^\circ_{\text{H(Pt)}}\cdot F\cdot n_{\text{e}^-}=-0,29654*96485*1=-28,61 \text{ kJ/mol}$$
 iekļaujoties Alberty datos. [8,15]



Veidošanās 41. no elementiem  $\text{O}_2\text{gas} + \text{H}_2\text{gas} + \text{H}_2\text{O} = \text{H}_2\text{O}_2\text{aq}$   $\Delta G^\circ_{\text{UnivAlbera}} = -134.03 \text{ kJ/mol}$ ;  $\Delta G^\circ_{\text{Albera}} = -48.39 \text{ kJ/mol}$ ;

$$\Delta G_{\text{H}_2\text{O}_2\text{Albera}} = G_{\text{H}_2\text{O}_2\text{aq}} - (G_{\text{O}_2\text{gas}} + G_{\text{H}_2\text{gas}} + G_{\text{H}_2\text{O}}) = \underline{284 - (85.64 + 303 + 0)} = -104.64 \text{ kJ/mol};$$

$\text{H}_2\text{O}_2\text{aqua}$  dismutācijas Nernsta pus reakcijās Red and Ox absolūto standarta brīvās enerģijas izmaiņu summa



$$\Delta G_{\text{EqStandartaAbsolūta}} = (E^\circ_{\text{H}_2\text{O}_2\text{aqRed}} - E^\circ_{\text{H}_2\text{O}_2\text{aqOx}}) * F * n = -238.5 \text{ kJ/mol};$$

$$\Delta G_{\text{Albera}} = G_{\text{O}_2\text{aqua}} + 2 * G_{\text{H}_2\text{O}} - 2 * G_{\text{H}_2\text{O}_2} = \underline{90.63 - 329.13} = -238.5 \text{ kJ/mol},$$

Reducēšana Nernsta:  $\text{H}_2\text{O}_2\text{aqua} + 2\text{H}_2\text{O} = \text{O}_2\text{aqua} + 2\text{H}_3\text{O}^+ + 2\text{e}^-$ ; absolūtais potenciāls  $E^\circ_{\text{H}_2\text{O}_2\text{aqRed}} = 0.4495 \text{ V}$  [20],

$$\Delta G_{\text{H}_2\text{O}_2\text{aqAlbera}} = G_{\text{O}_2\text{aq}} + 2G_{\text{H}_3\text{O}^+} - G_{\text{H}_2\text{O}_2} - 2G_{\text{H}_2\text{O}} = \underline{330 + 2 * 22.44 - 284.25 - 2 * 0} = \underline{100.38 \text{ kJ/mol}}$$

$$\Delta G_{\text{EqH}_2\text{O}_2} = E^\circ_{\text{H}_2\text{O}_2\text{aq}} * F * 2 = 0.4495 * 96485 * 2 = \underline{86.7 \text{ kJ/mol}}$$

Oksidēšana **inversais**  $\text{H}_2\text{O}_2 + 2\text{H}_3\text{O}^+ + 2\text{e}^- = 4\text{H}_2\text{O}$ ; absolūtais potenciāls  $-E^\circ_{\text{H}_2\text{O}_2\text{aqOx}} = -1.6855 \text{ V}$  Suhotina [18];

$$\Delta G_{\text{H}_2\text{O}_2\text{OxAlbera}} = 4 * G_{\text{H}_2\text{O}} - (G_{\text{H}_2\text{O}_2} + 2 * G_{\text{H}_3\text{O}^+}) = \underline{4 * 0 - (284.25 + 2 * 22.44)} = \underline{-319.38 \text{ kJ/mol}}$$

$$\Delta G_{\text{EqOxH}_2\text{O}_2} = -E^\circ_{\text{H}_2\text{O}_2\text{aqOx}} * F * 2 = -1.6855 * 96485 * 2 = \underline{-325.25 \text{ kJ/mol}};$$

$$\Delta G_{\text{EqStandarta}_2\text{H}_2\text{O}_2} = (E^\circ_{\text{H}_2\text{O}_2\text{aqRed}} - E^\circ_{\text{H}_2\text{O}_2\text{aqOx}}) * F * n = (0.4495 - 1.6855) * 96485 * 2 = (-1.236) * 96485 * 2 = \underline{-238.5 \text{ kJ/mol}};$$

$$\Delta G_{\text{Albera}_2\text{H}_2\text{O}_2} = G_{\text{O}_2\text{aqua}} + 2 * G_{\text{H}_2\text{O}} - 2 * G_{\text{H}_2\text{O}_2} = \underline{330 + 2 * 0 - 2 * G_{\text{H}_2\text{O}_2}} = \underline{-238.5 \text{ kJ/mol}};$$

$$G_{\text{H}_2\text{O}_2} = (G_{\text{O}_2\text{aqua}} + 2 * G_{\text{H}_2\text{O}} + \Delta G_{\text{Albera}_2\text{H}_2\text{O}_2}) / 2 = (330 + 2 * 0 + 238.5) / 2 = \underline{568.5 / 2} = \underline{284.25 \text{ kJ/mol}};$$

**Absolūtās** enerģijas saturs  $G_{\text{H}_2\text{O}_2} = \underline{284.25 \text{ kJ/mol}}$  ir noteikts uz nulles  $G_{\text{H}_2\text{O}} = G_{\text{CO}_2\text{gas}} = 0 \text{ kJ/mol}$  vielu fona. [8]

Veidošanās no elementiem  $\text{H}_2\text{gas} + \text{O}_2\text{gas} \Rightarrow \text{H}_2\text{O}_2$ ;  $\Delta G^\circ_{\text{UnivAlbera}} = -134.03 \text{ kJ/mol}$ ,  $\Delta G^\circ_{\text{Albera}} = -48.39 \text{ kJ/mol}$ :

$$\Delta G_{\text{Albera}} = G_{\text{H}_2\text{O}_2} - (G_{\text{O}_2\text{gas}} + G_{\text{H}_2\text{gas}}) = \underline{284.25 - (303 + 85.64)} = \underline{-104.4 \text{ kJ/mol}}. \text{ 41., 54. } \underline{\text{lapas}} [1, 8, 20]$$

Homeostāzes atraktori  $\text{pH} = 7.36$ ,  $[\text{H}_2\text{O}] = 55.3 \text{ M}$  pie peroksīda koncentrācijas viens. **Absolūtā** potenciālu skalā reducēšanas **absolūtā** un oksidēšanas **inversā** potenciālu summa  $(E_{\text{Red}} - E_{\text{Ox}}) = -1.26 \text{ V}$  uzrāda **absolūtās** brīvās enerģijas saturu vienā molā  $G_{\text{HomeostāzesH}_2\text{O}_2} = \underline{369.7 \text{ kJ/mol}}$ :

$$E_{\text{Red}} = E^\circ_{\text{RedH}_2\text{O}_2} + 0.0591/2 * \lg([\text{O}_2\text{aqua}] * [\text{H}_3\text{O}^+]^2 / [\text{H}_2\text{O}_2] / [\text{H}_2\text{O}]) = 0.4495 + 0.0591/2 * \lg(6 * 10^{-5} * 10^{(-7.36*2)} / 1 / 55.3^2) = -0.213 \text{ V}$$

$$-E_{\text{Ox}} = E^\circ_{\text{H}_2\text{O}_2\text{Ox}} + 0.0591/2 * \lg([\text{H}_2\text{O}_2] * [\text{H}_3\text{O}^+]^2 / [\text{H}_2\text{O}]^4) = -1.6855 + 0.0591/2 * \lg(1 * 10^{(-7.36*2)} / 55.3^4) = -2.3265 \text{ V}$$

$$\text{Homeostāzes: } \Delta G_{\text{EqBioChem}} = (E_{\text{Red}} - E_{\text{Ox}}) * F * n = (-0.2132 - 2.3265) * 96485 * 2 = (-2.5397) * 96485 * 2 = \underline{-490.1 \text{ kJ/mol}}$$

$$\Delta G_{\text{AlberaBioChem}} = G_{\text{O}_2\text{Biochem}_\text{arteria}} + 2 * G_{\text{H}_2\text{O}_2\text{BioChemistry}} - 2 * G_{\text{H}_2\text{O}_2} = \underline{78.08 + 2 * 85.64 - 2 * G_{\text{BioCHH}_2\text{O}_2}} = \underline{-490.1 \text{ kJ/mol}}; [8]$$

$$2 * G_{\text{H}_2\text{O}_2} = G_{\text{O}_2\text{Biochem}_\text{arteria}} + 2 * G_{\text{H}_2\text{O}_2\text{BioChemistry}} - \Delta G_{\text{Albera}} = \underline{78.08 + 2 * 85.64 + 490.1} = \underline{2 * 369.7} = \underline{739.5 \text{ kJ/mol}}$$

Peroksīda liela ātruma protolīzes  $\text{H}_2\text{O} + \text{H}_2\text{O}_2 = \text{H}_3\text{O}^+ + \text{HOO}^-$  līdzsvara konstante aprēķināta no  $\text{pK}_a = 11.75$ :

$$\underline{K_{\text{eqH}_2\text{O}_2} = K_a / [\text{H}_2\text{O}]} = [\text{H}_3\text{O}^+] [\text{HOO}^-] / [\text{H}_2\text{O}] [\text{H}_2\text{O}_2] = 10^{(-11.57)} / 55.3 = 10^{(-13.31)}, \text{ p}K_{\text{eqH}_2\text{O}_2} = 13.31. [1]$$

**Absolūtās** enerģijas izmaiņas minimums  $\underline{75.97 \text{ kJ/mol}}$  ļauj aprēķināt peroksīda anjona enerģiju molā  $G_{\text{HOO}^-}$ :

$$\Delta G_{\text{EqH}_2\text{O}_2} = -R * T * \ln(K_{\text{eqH}_2\text{O}_2}) = -8.3144 * 298.15 * \ln(10^{(-13.31)}) / 1000 = \underline{75.97 \text{ kJ/mol}}.$$

$$\Delta G_{\text{EqH}_2\text{O}_2} = G_{\text{H}_3\text{O}^+} + G_{\text{HOO}^-} - G_{\text{H}_2\text{O}} - G_{\text{H}_2\text{O}_2} = \underline{75.97 \text{ kJ/mol}}, \Delta G_{\text{EqH}_2\text{O}_2} = \underline{22.44 + G_{\text{HOO}^-} - 0 - 284.25} = \underline{75.97 \text{ kJ/mol}}.$$

Anjona enerģija molā ir  $G_{\text{HOO}^-} = \Delta G_{\text{EqH}_2\text{O}_2} + G_{\text{H}_2\text{O}} + G_{\text{H}_2\text{O}_2} - G_{\text{H}_3\text{O}^+} = \underline{-22.44 + 75.97 + 0 + 284.25} = \underline{337.8 \text{ kJ/mol}}$ .

Elektroķīmiska anjonu  $\text{HOO}^-$  oksidēšanas **absolūtais** standarta potenciāls ir  $E^\circ_{\text{HOO}^- \text{aqAlbera}} = 0.07587 \text{ Volts}$ . Oksidēšanas brīvās enerģijas izmaiņa ir pozitīva endoerģiska ar zemu **absolūto** standarta potenciālu:

$$\Delta G_{\text{HOO}^- \text{aqAlbera}} = G_{\text{O}_2\text{aq}} + G_{\text{H}_3\text{O}^+} - (G_{\text{HOO}^-} + G_{\text{H}_2\text{O}}) = \underline{330 + 22.44 - (337.8 + 0)} = \underline{14.64 \text{ kJ/mol}}.$$

$$\underline{\text{HOO}^- + \text{H}_2\text{O} = \text{O}_2\text{aqua} + \text{H}_3\text{O}^+ + 2\text{e}^-}; E^\circ_{\text{HOO}^- \text{aq}} = \Delta G_{\text{HOO}^- \text{aqAlbera}} / F / 2 = \underline{14640 / 96485 / 2} = \underline{0.07587 \text{ V}}.$$

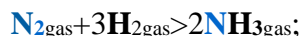
$$G_{\text{H}_2\text{O}_2} = \underline{284.25 \text{ kJ/mol}}; G_{\text{H}_3\text{O}^+} + G_{\text{HOO}^-} = 22.44 + \underline{337.8} = \underline{360.24 \text{ kJ/mol}}$$

Tabula 1. Nernsta pus- un inversās reakcijas	Standart potenciāli E° dati no [1-24]	Ūdens atlaide klasika E° <sub>H=0</sub>	Termodinamiskā skala 0,10166 V	Absolūtā -0,3982 V
$\text{OH}^- = \text{HO} + \text{e}^-$	CRC	2,020	2,122	1,7235
$4 \text{H}_2\text{O} = \text{H}_2\text{O}_{2\text{aqua}} + 2 \text{H}_3\text{O}^+ + 2 \text{e}^-$	Suchotina	1,776	2,0837	1,6855
$\text{H}_2\text{O}_2 + 2 \text{H}_2\text{O} = \text{O}^{2\text{aqua}} + 2 \text{H}_3\text{O}^+ + \text{e}^-$	David Harris	1,276	1,4811	1,0829
$6\text{H}_2\text{O} = \text{O}_{2\text{g}} + \text{H}_2\text{O} + 4\text{H}_3\text{O}^+ + 4 \text{e}^-$ ; $5\text{H}_2\text{O} = \text{O}_{2\text{aq}} + 4\text{H}_3\text{O}^+ + 4 \text{e}^-$ ;		1,2288	1,45814	1,0868
$\text{HNO}_2 + 4\text{H}_2\text{O} = \text{NO}_3^- + 3\text{H}_3\text{O}^+ + 2\text{e}^-$	University Alberta	0,928	1,2352	0,8370
$\text{NO}_2^- + 3 \text{H}_2\text{O} = \text{NO}_3^- + 2 \text{H}_3\text{O}^+ + 2\text{e}^-$	David Harris	0,835	1,0913	0,6931
<b>Hydroquinone</b> + $2\text{H}_2\text{O} = \text{p-quinone} + 2\text{H}_3\text{O}^+ + 2\text{e}^-$		0,699	0,9041	0,5059
$\text{H}_2\text{O}_{2\text{aqua}} + 2\text{H}_2\text{O} = \text{O}_{2\text{aqua}} + 2\text{H}_3\text{O}^+ + 2\text{e}^-$	University Alberta	0,695	0,8477	0,4495
$\text{H}_2\text{O}_{2\text{aqua}} + \text{H}_2\text{O} = \text{O}_{2\text{aqua}} + \text{H}_3\text{O}^+ + \text{H}^-(\text{H}^+ + 2\text{e}^-)$	University Alberta	0,695	0,8477	0,4495
$\text{Fe}^{2+} = \text{Fe}^{3+} + \text{e}^-$	University Alberta	0,769	0,8707	0,4725
<b>Ubiquinol</b> + $2\text{H}_2\text{O} = \text{Ubiquinone} + 2\text{H}_3\text{O}^+ + 2\text{e}^-$		0,459	0,6638	0,2656
<b>Succinate</b> <sup>2-</sup> + $2\text{H}_2\text{O} = \text{Fumarate}^{2-} + 2\text{H}_3\text{O}^+ + 2\text{e}^-$ pH=7 E <sub>0</sub> =0,031 V		0,4447	0,6494	0,2512
<b>ButyrylCoA</b> + $2\text{H}_2\text{O} = \text{CrotonylCoA} + 2\text{H}_3\text{O}^+ + 2\text{e}^-$		0,399	0,6038	0,2056
<b>AscorbicAcid</b> + $2\text{H}_2\text{O} = \text{C}_6\text{H}_6\text{O}_6 + 2\text{H}_3\text{O}^+ + 2\text{e}^-$ DC, Harris		0,390	0,5947	0,1965
<b>glycolate</b> + $2\text{H}_2\text{O} = \text{Glyoxylate} + \text{H}^-(\text{H}^+ + 2\text{e}^-) + \text{H}_3\text{O}^+$ ; D.C.Harris		0,324	0,5287	0,1305
$\text{C}_6\text{H}_{12}\text{O}_6 + 4\text{H}_2\text{O} = 2\text{H}_3\text{O}^+ + 6\text{H}_3\text{O}^+ + 6\text{HCO}_3^- + 24\text{e}^-$ <a href="#">6. lapa</a> Kaksis		0,4089	0,51054	0,1392
$\text{HO}_2^- + \text{H}_2\text{O} = \text{O}_{2\text{aqua}} + \text{H}_3\text{O}^+ + 2\text{e}^-$	Aris Kaksis	-	-	0,07587
$\text{Fe}^{2+} = \text{Cytochrome F Fe}^{3+} + \text{e}^-$	David Harris	0,365	0,4667	0,0685
$[\text{Fe}^{\text{II}}(\text{CN})_6]^{4-} = [\text{Fe}^{\text{III}}(\text{CN})_6]^{3-} + \text{e}^-$	University Alberta	0,356	0,4574	0,0592
<b>Malate</b> <sup>2-</sup> + $2\text{H}_2\text{O} = \text{Oxalo-acetate}^{2-} + 2\text{H}_3\text{O}^+ + 2\text{e}^-$		0,248	0,4528	0,0546
$\text{Fe}^{2+} = \text{Cytochrome a3 Fe}^{3+} + \text{e}^-$		0,350	0,4517	0,0535
<b>Lactate</b> <sup>-</sup> + $2\text{H}_2\text{O} = \text{Pyruvate}^- + \text{H}_3\text{O}^+ + \text{H}^-(\text{H}^+ + 2\text{e}^-)$		0,229	0,3823	-0,0159
<b>FADH<sub>2</sub></b> + $2\text{H}_2\text{O} = \text{FADfree} + 2\text{H}_3\text{O}^+ + 2\text{e}^-$		0,195	0,3998	0,0016
<b>CH<sub>3</sub>COO<sup>-</sup></b> + $2\text{H}_2\text{O} = \text{glycolate} + \text{H}^-(\text{H}^+ + 2\text{e}^-) + \text{H}_3\text{O}^+$ ; D.C.Harris		0,161	0,3652	-0,0330
$\text{H}_2\text{S}_{\text{aq}} + 2\text{H}_2\text{O} = \text{S}_{\text{rombisks}} + 2\text{H}_3\text{O}^+ + 2\text{e}^-$ ;	CRC 2010	0,142	0,3467	-0,0515
<b>CH<sub>3</sub>CH<sub>2</sub>OH</b> + $2\text{H}_2\text{O} = \text{CH}_3\text{CHO} + \text{H}_3\text{O}^+ + \text{H}^-(\text{H}^+ + 2\text{e}^-)$ KortlyShucha		0,190	0,3432	-0,0550
$\text{Fe}^{2+} = \text{Cytochrome a Fe}^{3+} + \text{e}^-$		0,2900	0,3917	-0,0065
<b>2GlutathSH</b> + $2\text{H}_2\text{O} = \text{GlutaS-Sthione} + 2\text{H}_3\text{O}^+ + 2\text{e}^-$		0,1841	0,3888	-0,0094
<b>HSH</b> + $2\text{H}_2\text{O} = \text{Srhb} + 2\text{H}_3\text{O}^+ + 2\text{e}^-$	University Alberta	0,1739	0,3786	-0,0196
$\text{Fe}^{2+} = \text{Cytochrome c Fe}^{3+} + \text{e}^-$		0,2540	0,3557	-0,0425
<b>LipSHSH</b> + $2\text{H}_2\text{O} = \text{LipoicAcidS-S} + 2\text{H}_3\text{O}^+ + 2\text{e}^-$		0,1241	0,3288	-0,0694
$\text{Fe}^{2+} = \text{Cytochrome c1 Fe}^{3+} + \text{e}^-$		0,2200	0,3217	-0,0765
<b>β-OH Butyrate</b> <sup>-</sup> + $2\text{H}_2\text{O} = \text{AcetoAcetate}^- + 2\text{H}_3\text{O}^+ + 2\text{e}^-$		0,0681	0,2728	-0,1254
<b>isocitrate</b> <sup>2-</sup> + $2\text{H}_2\text{O} = \alpha\text{-Ketoglutarate}^{2-} + \text{CO}_2 + 2\text{H}_3\text{O}^+ + 2\text{e}^-$		0,0341	0,2388	-0,1594
<b>Nernst's</b> $\text{H}_{2\text{aq}} + 2\text{H}_2\text{O} = 2\text{H}_3\text{O}^+ + 2\text{e}^-$ Kaksis $\Delta G_{\text{Hess, H}_3\text{O}^+} = -58,12$ kJ/mol		Oksidēšana ar grafīta elektrodu		-0,3020
<b>Inverse:</b> $2\text{H}_3\text{O}^+ + 2\text{e}^- = \text{H}_{2\text{aq}} + 2\text{H}_2\text{O}$ ; $\Delta G_{\text{Hess, H}_{2\text{aq}}} = 58,12$ kJ/mol		Reducēšana ar grafīta elektrodu		0,3020
$2\text{H}(\text{Pt}) + \text{H}_2\text{O} = \text{H}_{2\text{aq}}$ $\Delta G_{\text{Alberty, šķ. H}(\text{Pt})} = G_{\text{H}_{2\text{aq}}} - 2G_{\text{H}(\text{Pt})} - G_{\text{H}_2\text{O}} = 1,14$ kJ/mol		$K_{\text{šķ. H}(\text{Pt})} = \frac{[\text{H}(\text{Pt})]^2 \cdot [\text{H}_2\text{O}]}{[\text{H}_{2\text{aq}}]} = 0.631$		
$\text{H}(\text{Pt}) + \text{H}_2\text{O} = \text{H}_3\text{O}^+ + (\text{Pt}) + \text{e}^-$ ; $[\text{H}_3\text{O}^+] = 1 \text{ M}$ pH=0 classic zero		<b>0,0</b> ; $[\text{H}_2\text{SO}_4] = 1 \text{ M}$	<b>0,10166</b>	<b>-0,2965</b>
<b>Luciferin</b> + $\text{OH}^- = ?\text{luciferin} + \text{CO}_2\text{aqua} + \text{OH}^- + 3\text{H}(3\text{H}^+ + 3\text{e}^-) + \text{e}^-$ ;		0,0000	0,1017	-0,2965
$\text{Fe}^{2+} = \text{Cytochrome b Fe}^{3+} + \text{e}^-$		0,0770	0,1787	-0,2195
<b>CH<sub>3</sub>CHO</b> + $3\text{H}_2\text{O} = \text{CH}_3\text{COOH} + 2\text{H}_3\text{O}^+ + 2\text{e}^-$ Suchotina		-0,1180	0,1382	-0,2600
<b>Glycaldeh3P<sup>2-</sup></b> + $2\text{H}_2\text{O} + \text{HPO}_4^{2-} = 13\text{PGlycerate}^{4-} + \text{H}_3\text{O}^+ + \text{H}^-$		-0,1314	0,0218	-0,3764
<b>NADPH</b> = $\text{NADP}^+ + \text{H}^-(\text{H}^+ + 2\text{e}^-)$ ;		-0,1170	-0,0153	-0,4135
<b>NADH</b> = $\text{NAD}^+ + \text{H}^-(\text{H}^+ + 2\text{e}^-)$ ;	David Harris	-0,1130	-0,0113	-0,4095
$\text{O}^{2\text{aqua}} = \text{O}_{2\text{aqua}} + \text{e}^-$	Suchotina	-0,2450	-0,1433	-0,5415
<b>Ferredoxin</b> $\text{Fe}^{2+} = \text{Ferredoxin Fe}^{3+} + \text{e}^-$		-0,4320	-0,3303	-0,7285
$\text{C}_6\text{H}_{12}\text{O}_6 + 4\text{H}_2\text{O} = 2\text{C}_3\text{H}_4\text{O}_3 + 4\text{H}_3\text{O}^+ + 4\text{e}^-$ Stryer		-0,5427	-0,3380	-0,7362
$\text{S}^{2-} = \text{S}_{\text{rombisks}} + 2 \text{e}^-$ ;	CRC 2010	-0,4763	-0,3746	-0,7728
$\text{HS}^- + \text{OH}^- = \text{S}_{\text{rombisks}} + \text{H}_2\text{O} + 2\text{e}^-$ ;	CRC 2010	-0,4780	-0,3248	-0,7230
$\text{H}(\text{Pt}) + \text{OH}^- = \text{H}_2\text{O} + \text{e}^-$	Suchotina	-0,8280	-0,6233	-1,0215
<b>Ubiquinol6</b> + $2\text{H}_2\text{O} = \text{Ubiquinone6} + 2\text{H}_3\text{O}^+ + 2\text{e}^-$ CRC 2012		-1,0500	-0,8453	-1,2435

**Potenciālu skalas** noteikšanas ūdens uzskaites un ūdeņraža elektroda korekcija uz **Absolūto skalu** piemērs. Klasiska ūdens atlaide Nernsta skābekļa pus reakcijai:  $6\text{H}_2\text{O}=\text{O}_{2\text{aqua}}+4\text{H}_3\text{O}^++4\text{e}^-$   $E^\circ_{\text{ozklasika}}=1,229\text{ V}$ . [18] Ūdens uzskaites potenciāls:  $E^\circ_{6\text{H}_2\text{O}}=E^\circ_{\text{ozklasika}}-0,0591/4\cdot\log(1/[\text{H}_2\text{O}]^6)=1,229-0,014775\cdot\log(1/55,3^6)=1,383\text{ V}$ . Hydrogen electrode correction +0,10166:  $E^\circ_{\text{ozTermodinamika}}=E^\circ_{6\text{H}_2\text{O}}+0,10166=1,383+0,10166=1,485\text{ Volts}$ . **Absolūtā standarta potenciālu skala** ir  $E^\circ_{\text{ozAbsolūtā}}=E^\circ_{\text{ozTermodinamika}}-0,3982=1,485-0,3982=1,0868\text{ Volts}$ .

Veidošanās no elementiem  $\text{N}_{2\text{gas}}+3\text{H}_{2\text{gas}}>2\text{NH}_{3\text{gas}}$  absolūtā enerģija ir  $G_{\text{N}_{2\text{gas}}}=107,28\text{ kJ/mol}$ ; ;  $G_{\text{NH}_{3\text{gas}}}=165,7\text{ kJ/mol}$  ; Classic Hess elements have zero  $2\Delta G_{\text{Hess\_NH}_{3\text{gas}}}=2G^\circ_{\text{NH}_{3\text{gas}}}-G^\circ_{\text{N}_{2\text{gas}}}+3G^\circ_{\text{H}_2}=2\cdot-16,4-(0+3\cdot0)=-32,8\text{ kJ/mol}$  . [1] Alberty elementa ūdeņraža  $G_{\text{H}_2\text{gas}}=85,64\text{ kJ/mol}$  **absolūtā** enerģija ar Hesa veidošanos  $-32,8\text{ kJ/mol}$  aprēķina slāpekļa **absolūto** enerģiju  $G_{\text{N}_{2\text{gas}}}=2G_{\text{NH}_{3\text{gas}}}-2\Delta G_{\text{Hess\_NH}_{3\text{gas}}}+3G_{\text{H}_2\text{gas}}=2\cdot165,7-(2\cdot-16,4+3\cdot85,64)=107,28\text{ kJ/mol}$ ; [8]  $\Delta G_{\text{HessFormationN}_{2\text{aqua}}}=G_{\text{N}_{2\text{aqua}}}-G_{\text{N}_{2\text{gas}}}+G_{\text{H}_2\text{O}}=18,7-(107,28+0)=-88,5\text{ kJ/mol}$ ; [8]  $G_{\text{N}_{2\text{gas}}}=G^\circ_{\text{N}_{2\text{aqua}}}-\Delta G_{\text{Hess\_šk\_N}_{2\text{aqua}}}+G_{\text{H}_2\text{O}}=18,7-(-88,5+0)=107,2\text{ kJ/mol}$ ; [8] [Alberty](#)

Substanc e	$\Delta H^\circ_{\text{H}}\text{ kJ/mol}$	$\Delta S^\circ_{\text{H}}\text{ J/mol/K}$	$\Delta G^\circ_{\text{H}}\text{ kJ/mo}$ l
$\text{NH}_{3\text{gas}}$	-45,9	192,77	-16,4
$\text{NH}_{3\text{gas}}$			<b>438,85</b>
$\text{NH}_{3\text{aq}}$	-132,5608	-739,2922	<b>91,1056</b>
$\text{N}_{2\text{gas}}$	$G_{\text{N}_{2\text{gas}}}=$	-15,26	<b>107,2</b>
$\text{N}_{2\text{aq}}$	-10,54	<b>98,1</b>	<b>18,7</b>



$$G_{\text{N}_{2\text{gas}}}=2\cdot165,6593-(-32,8+3\cdot85,64)=107,2\text{ kJ/mol}; [8] \text{ [Alberty](#)};$$

$$G_{\text{N}_{2\text{gas}}}=2G_{\text{NH}_{3\text{gas}}}-2\Delta G_{\text{Hess\_NH}_{3\text{gas}}}+3G_{\text{H}_2\text{gas}}=107,2\text{ kJ/mol}; [8] \text{ [Alberty](#)};$$

Simts gramos ūdens izšķīst  $0,00175\text{ g}/100\text{g\_H}_2\text{O}$  slāpekļa gāzes ar blīvumu  $996\text{ g/L}$ .

Šķīdība  $[\text{N}_{2\text{aqua}}]=0,00175/100,00175\cdot996=0,01743/28,02=10^{-3,206}\text{ M}$  un šķīdības konstante ir:

$$K_{\text{šk}}=10^{-(3,206)}/[\text{H}_2\text{O}]=10^{-(3,206)}/55,3=10^{-4,949}; \Delta G_{\text{šk}}=-R\cdot T\cdot\ln(K_{\text{šk}})=-8,3144\cdot298,15\cdot\ln(10^{-(4,949)})=28,25\text{ kJ/mol}.$$

Mols brīvās enerģijas ir  $G_{\text{N}_{2\text{gas}}}=G_{\text{N}_{2\text{aqua}}}-\Delta G_{\text{Hess\_šk\_N}_{2\text{aqua}}}+G_{\text{H}_2\text{O}}=18,7-(28,25+0)=-9,55\text{ kJ/mol}$ ; CRC 2010 [1,8]

Šķīdības  $\text{N}_{2\text{gas}}+\text{H}_2\text{O}+\Delta G=\text{N}_{2\text{aq}}+\text{Q}$ ;  $G_{\text{N}_{2\text{gas}}}=-9,55\text{ kJ/mol}$  brīvās enerģijas izmaiņa ir:

$$\Delta G_{\text{Hess\_šk\_N}_{2\text{aqua}}}=G_{\text{N}_{2\text{aqua}}}-G_{\text{N}_{2\text{gas}}}+G_{\text{H}_2\text{O}}=18,7-(-9,55+0)=28,25\text{ kJ/mol}$$
. CRC 2010 [1,8] [Alberty](#)

Šķīdības konstante ir  $K_{\text{šk}}=[\text{N}_{2\text{aqua}}]/[\text{H}_2\text{O}]=10^{-(3,206)}/55,3=10^{-4,949}$ , kuras brīvās enerģijas izmaiņas minimums ir  $\Delta G_{\text{šk}}=-R\cdot T\cdot\ln(K_{\text{šk}})=-8,3144\cdot298,15\cdot\ln(10^{-(4,949)})=28,25\text{ kJ/mol}$ .

Hesa brīvās enerģijas izmaiņa ir sakrītoša ar

$$\Delta G_{\text{Hess\_šk\_N}_{2\text{aqua}}}=G_{\text{N}_{2\text{aqua}}}-G_{\text{N}_{2\text{gas}}}+G_{\text{H}_2\text{O}}=18,7-(107,28-0)=28,25\text{ kJ/mol}$$
.

Slāpekļa gāzes brīvās enerģijas saturs izteiksmē

$$G_{\text{N}_{2\text{gas}}}=G_{\text{N}_{2\text{aqua}}}-\Delta G_{\text{Hess\_šk\_N}_{2\text{aqua}}}+G_{\text{H}_2\text{O}}=18,7-(28,25+0)=-9,55\text{ kJ/mol}$$
 ir negatīvs.

Solubility  $\text{NH}_{3\text{gas}}+\text{H}_2\text{O}+\Delta G\rightleftharpoons\text{NH}_{3\text{aq}}+\text{Q}$ ;  $G_{\text{NH}_{3\text{aq}}}=91,1\text{ kJ/mol}$ ;

$$\Delta H_{\text{Hydration}}=\Delta H^\circ_{\text{NH}_{3\text{aq}}}-\Delta H^\circ_{\text{NH}_{3\text{gas}}}-\Delta H^\circ_{\text{H}_2\text{O}}=-132,5608+45,94-286,65=373,3\text{ kJ/mol};$$

$$S_{\text{Hydration}}=\Delta S^\circ_{\text{NH}_{3\text{aq}}}+\Delta S^\circ_{\text{H}_2\text{O}}-\Delta S^\circ_{\text{NH}_{3\text{gas}}}=-739,2922-192,77-69,9565=-1002\text{ J/mol/K};$$

$$\Delta G_{\text{Hess\_NH}_{3\text{gas}}}=\Delta H_{\text{Hydrations}}-T\cdot\Delta S_{\text{Hydration}}=-373,3-298,15\cdot-1,002=-74,5537\text{ kJ/mol};$$

$$K_{\text{šk}}=\exp(-\Delta G_{\text{Hydration}}/R/T)=\exp(74553,7/8,3144/298,15)=10^{13,06}$$

$$G_{\text{NH}_{3\text{gas}}}=\Delta G_{\text{NH}_{3\text{aq}}}-\Delta G_{\text{Hess\_šk\_NH}_{3\text{gas}}}+G_{\text{H}_2\text{O}}=91,1056-(-74,5537+0)=165,7\text{ kJ/mol}; [8] \text{ [Alberty](#)};$$

$$G_{\text{NH}_{3\text{gas}}}=(2\Delta G_{\text{Hess\_NH}_{3\text{gas}}}+(G_{\text{N}_{2\text{gas}}}+3G_{\text{H}_2})) / 2 = (-32,8+(107,2+3\cdot85,64)) / 2 = 165,7\text{ kJ/mol}; \text{ Hess [1,8] Alberty}$$

$$G_{\text{NH}_{3\text{gas}}}=\Delta G^\circ_{\text{NH}_{3\text{aq}}}-\Delta G_{\text{Hess\_šk\_NH}_{3\text{gas}}}-G^\circ_{\text{H}_2\text{O}}=91,1056-(-74,5537)-(-0)=165,7\text{ kJ/mol}; [8] \text{ [Alberty](#)};$$

$$G_{\text{NH}_{3\text{gas}}}=\Delta G^\circ_{\text{NH}_{3\text{aq}}}-\Delta G_{\text{Hess\_NH}_{3\text{gas}}}-G_{\text{H}_2\text{O}}=91,1056-(-74,5537)-(-273,19)=438,85\text{ kJ/mol}; \text{ CRC 2010}$$

Vājas skābes protolīzes norise  $\text{NH}_4^++\text{H}_2\text{O}=\text{NH}_{3\text{aq}}+\text{H}_3\text{O}^+$ ;  $pK_{\text{eq}}=10,99$ ; uzrāda enerģiju  $G_{\text{NH}_4^+}=232,9\text{ kJ/mol}$ ,  $\Delta G_{\text{eq}}=-R\cdot T\cdot\ln(K_{\text{eq}})=-8,3144\cdot298,15\cdot\ln(10^{-(10,99)})=G_{\text{NH}_3\text{Hydration}}+G_{\text{H}_3\text{O}}-G_{\text{NH}_4^+}-G_{\text{H}_2\text{O}}=62,76\text{ kJ/mol}$ , [16<sup>th</sup> page](#):

$$\Delta G_{\text{eq}}=G_{\text{NH}_{3\text{aq}}}+G_{\text{H}_3\text{O}}-G_{\text{NH}_4^+}-G_{\text{H}_2\text{O}}=91,1+22,44-G_{\text{NH}_4^+}-0=62,75\text{ kJ/mol},$$

$$G_{\text{NH}_4^+}=G_{\text{NH}_{3\text{aq}}}+G_{\text{H}_3\text{O}}-\Delta G_{\text{eq}}-G_{\text{H}_2\text{O}}=91,1+22,44-62,75-0=232,9\text{ kJ/mol},$$

$K_{\text{eq}3}$ ; protolīze  $\text{NH}_4^++\text{H}_2\text{O}+\Delta G+\text{Q}=\text{NH}_{3\text{aq}}+\text{H}_3\text{O}^+$ ;  $pK_{\text{eq}}=10,9944$ ;  $\text{NH}_4^+=\text{H}^++\text{NH}_{3\text{aq}}$ ;  $pK_{\text{a}}=9,25$ ;

$$K_{\text{eq}3}=[\text{NH}_{3\text{aq}}]\cdot[\text{H}_3\text{O}^+]/[\text{NH}_4^+][\text{H}_2\text{O}]=\exp(-\Delta G_{\text{Hydration}}/R/T)=\exp(-62755,6/8,3144/298,15)=10^{-10,994};$$

$$\Delta G_{\text{eq}3}=-R\cdot T\cdot\ln(K_{\text{eq}})=-8,3144\cdot298,15\cdot\ln(1,013\cdot10^{-11})=62,75\text{ kJ/mol};$$

$$K_{\text{eq}3}=[\text{NH}_{3\text{aq}}]\cdot[\text{H}_3\text{O}^+]/[\text{NH}_4^+][\text{H}_2\text{O}]=[\text{H}_2\text{O}]\cdot K_{\text{H}_2\text{O}}/K_{\text{NH}_4\text{OH}}=55,3\cdot3,26\cdot10^{-(18)}/1,78/10^{-(5)}=1,013\cdot10^{-(11)};$$

$$\Delta G_{\text{Hydration}}=\Delta G_{\text{NH}_{3\text{aq}}}-\Delta G_{\text{NH}_{3\text{gas}}}-G_{\text{H}_2\text{O}}=91,1056-(-16,4-0)=107,5\text{ kJ/mol};$$

$$G_{\text{NH}_{3\text{aq}}}=\Delta G_{\text{Hydration}}+G_{\text{NH}_{3\text{gas}}}+G_{\text{H}_2\text{O}}=107,5+165,7+0=273,2\text{ kJ/mol};$$

**Tabula 2. Nernsta pus reakciju Standarta Electrodu Potenciāli klssikais, termodinamiskais absolūtais V.**

	Reducētā forma = Oksidētā forma	H <sub>2</sub> O atlaide klasika nulle E <sub>OH</sub> =0	Termodinamiskā. skala E <sub>OH</sub> =0,10166 V	Absolūtā skala -0,3982 V
<b>N</b>	$\text{NO}_2^- + 2\text{OH}^- = \text{NO}_3^- + \text{H}_2\text{O} + 2\text{e}^-$ ; pH>3,15 Suchotina [17]	0.01	0,0602	-0,3380
	$\text{HNO}_2 + 4\text{H}_2\text{O} = \text{NO}_3^- + 3\text{H}_3\text{O}^+ + 2\text{e}^-$ ; pH<3,15 Kortly, Shucha	0.94	1,2477	0,8495
	$\text{NO}_{\text{aq}} + 6\text{H}_2\text{O} = \text{NO}_3^- + 4\text{H}_3\text{O}^+ + 3\text{e}^-$ ; pH>3,15 Kortly, Shucha	0.96	1,1777	0,7795
	$\text{NH}_4^+ + 13\text{H}_2\text{O} = \text{NO}_3^- + 10\text{H}_3\text{O}^+ + 8\text{e}^-$ ; Suchotina	0.87	1,139027	0,740827
<b>Br</b>	$2\text{Br}^- = \text{Br}_2(\text{aq}) + 2\text{e}^-$ ; CRC	1,0873	1,18896	0,79076
<b>Bi</b>	$\text{Bi O}^+ + 6\text{H}_2\text{O} = \text{BiO}_3^- + 4\text{H}_3\text{O}^+ + 2\text{e}^-$ ; Suchotina	1,80	2,210645	1,812445
<b>Mn H<sup>+</sup></b>	$\text{Mn}^{2+} + 12\text{H}_2\text{O} = \text{MnO}_4^- + 8\text{H}_3\text{O}^+ + 5\text{e}^-$ ; Kortly, Shucha [18]	1,51	1,858848	1,460648
	$\text{MnO}_2 \downarrow + 4\text{OH}^- = \text{MnO}_4^- + 2\text{H}_2\text{O} + 3\text{e}^-$ ; Suchotina	0,603	0,635997	0,237797
	$\text{MnO}_4^{2-} = \text{MnO}_4^- + \text{e}^-$ ; Suchotina	0,558	0,65966	0,26146
<b>Pb</b>	$\text{Pb}^{2+} + 6\text{H}_2\text{O} = \text{PbO}_2(\text{s}) + 4\text{H}_3\text{O}^+ + 2\text{e}^-$ ; Kortly, Shucha [18]	1,455	1,865645	1,467445
	$\text{H}_2\text{SO}_3 + 4\text{H}_2\text{O} = \text{HSO}_4^- + 3\text{H}_3\text{O}^+ + 2\text{e}^-$ ; Suchotina pH<1,9	0,172	0,47965	0,08145
	$\text{HSO}_3^- + 4\text{H}_2\text{O} = \text{SO}_4^{2-} + 3\text{H}_3\text{O}^+ + 2\text{e}^-$ ; Suchotina 2=<pH<7	0,172	0,47965	0,08145
	$\text{SO}_3^{2-} + 2\text{OH}^- = \text{SO}_4^{2-} + \text{H}_2\text{O} + 2\text{e}^-$ ; Suchotina pH > 7	-0,93	-0,87984	-1,27804
	$\text{S}^{2-} = \text{S}(\text{s}) + 2\text{e}^-$ ; Kortly, Shucha	-0,48	-0,37834	-0,77654
	$\text{H}_2\text{S} + 2\text{H}_2\text{O} = \text{S}(\text{s}) + 2\text{H}_3\text{O}^+ + 2\text{e}^-$ ; Kortly, Shucha	0,141	0,345655	-0,05254
	$2\text{S}_2\text{O}_3^{2-} = \text{S}_4\text{O}_6^{2-} + 2\text{e}^-$ ; Suchotina	0,08	0,18166	-0,2165
<b>Fe</b>	$\text{Fe}^{2+} = \text{Fe}^{3+} + \text{e}^-$ ; Suchotina [18]	0,769	0,8717	0,4735
	$\text{Fe}(\text{s}) + \text{H}_2\text{O} = \text{Fe}^{2+} + 2\text{e}^-$ ; Suchotina	-0,4402	-0,2870	-0,6852
<b>Ag</b>	$\text{Ag} + \text{H}_2\text{O} = \text{Ag}^+ + \text{e}^-$ ; Kortly, Shucha [18]	0,7994	1,0041	0,6059
	$\text{Ag}(\text{s}) + \text{Cl}^- = \text{AgCl}(\text{s}) + \text{H}_2\text{O} + \text{e}^-$ ; Kortly, Shucha	0,2223	0,2210	-0,1772
	$\text{Ag} + 2\text{NH}_3(\text{aq}) = \text{Ag}(\text{NH}_3)_2^+ + \text{e}^-$ ; Suchotina	0,373	0,4747	0,0765
	$2\text{Ag} + 2\text{OH}^- = \text{Ag}_2\text{O}(\text{s}) + \text{H}_2\text{O} + 2\text{e}^-$ ; Suchotina	0,345	0,3952	-0,0030
<b>I</b>	$3\text{I}^- = \text{I}_3^- + 2\text{e}^-$ ; Kortly, Shucha	0,6276	0,72926	0,33106
<b>Cu</b>	$\text{Cu}(\text{Hg}) + \text{H}_2\text{O} = \text{Cu}^{2+} + (\text{Hg}) + 2\text{e}^-$ ; Kortly, Shucha	0,3435	0,4967	0,0985
<b>F</b>	$2\text{F}^- = \text{F}_2(\text{g}) + 2\text{e}^-$ ; Kortly, Shucha	2,87	2,97166	2,5735
<b>Cl</b>	$2\text{Cl}^- = \text{Cl}_2(\text{g}) + 2\text{e}^-$ ; Kortly, Shucha	1,358	1,45966	1,06146
	$\text{Cl}_2(\text{g}) + 4\text{H}_2\text{O} = 2\text{HOCl} + 2\text{H}_3\text{O}^+ + 2\text{e}^-$ ; Kortly, Shucha	1,63	1,93765	1,53945
<b>Cr</b>	$2\text{Cr}^{3+} + 21\text{H}_2\text{O} = \text{Cr}_2\text{O}_7^{2-} + 14\text{H}_3\text{O}^+ + 6\text{e}^-$ ; Kortly, Shucha	1,33	1,7921	1,3939
	$\text{Cr}^{3+} + 11\text{H}_2\text{O} = \text{HCrO}_4^- + 7\text{H}_3\text{O}^+ + 3\text{e}^-$ ; Kortly, Shucha	1,20	1,6793	1,2811
	$\text{Cr}(\text{OH})_3 \downarrow + 5\text{OH}^- = \text{CrO}_4^{2-} + 4\text{H}_2\text{O} + 3\text{e}^-$ ; pH>9; Suchotina [17]	-0,13	-0,1657	-0,5639
<b>C</b>	$\text{H}_2\text{C}_2\text{O}_4 + 2\text{H}_2\text{O} = 2\text{CO}_2 + 2\text{H}_3\text{O}^+ + 2\text{e}^-$ ; Suchotina	-0,49	-0,28534	-0,6835
<b>Cr</b>	$\text{Cr} + \text{H}_2\text{O} = \text{Cr}^{3+} + 3\text{e}^-$ ; Suchotina	-0,744	-0,6080	-1,0062
<b>Zn</b>	$\text{Zn} + \text{H}_2\text{O} = \text{Zn}^{2+} + 2\text{e}^-$ ; Kortly, Shucha	-0,7628	-0,6096	-1,0078

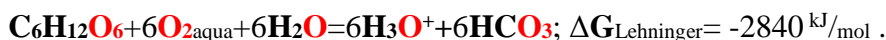
**Glc** 6. lpp. veidošanās no elementiem  $6\text{C} + 6\text{H}_2\text{gas} + 3\text{O}_2\text{gas} = \text{C}_6\text{H}_{12}\text{O}_6$  brīvās enerģijas izmaiņu aprēķina no Alberty

$$\text{datiem } \Delta G^\circ_{\text{Alberty}} = G_{\text{C}_6\text{H}_{12}\text{O}_6} - (6G_{\text{Cgraph}} + 6G_{\text{H}_2\text{gas}} + 3G_{\text{O}_2\text{gas}}) = -402,05 \text{ kJ/mol};$$

$$\Delta G^\circ_{\text{Alberty}} + (6G_{\text{Cgraph}} + 6G_{\text{H}_2\text{gas}} + 3G_{\text{O}_2\text{gas}}) = -402,05 + (6 \cdot 91,26 + 6 \cdot 85,6 + 3 \cdot 303) = G_{\text{C}_6\text{H}_{12}\text{O}_6} = 1568 \text{ kJ/mol};$$

**Glikoze (Glc)**  $\text{C}_6\text{H}_{12}\text{O}_6$  ar biokīmisko ūdeni  $6\text{H}_2\text{O}$  un skābekls  $6\text{O}_2\text{aqua}$  reducējas radot enerģijaas izmaiņu  $\Delta G_{\text{Lehninger}} = -2840 \text{ kJ/mol}$  un producējot  $6\text{HCO}_3^-$  un  $6\text{H}_3\text{O}^+$  jonus ģenerē koncentrācijas gradientus abpus membrānām darbinot osmozi un jonu transportu cauri akvaporīnu, bikarbonāta un protonu kanāliem membrānās:

Brīvā enerģija glikozei (**Glc**)  $G_{\text{C}_6\text{H}_{12}\text{O}_6}$  kvazi līdzsvaram aprēķināta lietojot Lehningera datus [6] oksidēšanā:



Enerģija  $-2840 = G_{\text{C}_6\text{H}_{12}\text{O}_6} - 6G_{\text{O}_2\text{Homeostāzes\_arterial}} - 6G_{\text{H}_2\text{O\_Biochem}} + (6G_{\text{H}_3\text{O}^+} + 6G_{\text{HCO}_3^-})$  ļauj izteikt glikozes

$G_{\text{C}_6\text{H}_{12}\text{O}_6} = 2840 - 6G_{\text{O}_2\text{Homeostāzes\_arterial}} - 6G_{\text{H}_2\text{O\_Biochem}} + (6G_{\text{H}_3\text{O}^+} + 6G_{\text{HCO}_3^-})$  kvazi līdzsvara standarta brīvās

enerģijas saturu  $G_{\text{StandardC}_6\text{H}_{12}\text{O}_6} = 2840 - 6 \cdot 330 - 6 \cdot 85,64 + 6 \cdot (22,44 + 46,08) = 757,28 \text{ kJ/mol}$  un

brīvās enerģijas izmaiņu homeostāzē  $G_{\text{C}_6\text{H}_{12}\text{O}_6} = 2840 - 6 \cdot 78,08 - 6 \cdot 85,64 + 6 \cdot (22,44 + 46,08) = 2268,8 \text{ kJ/mol}$ . Glikozes

brīvā enerģija ir standarta Alberty  $G_{\text{C}_6\text{H}_{12}\text{O}_6} = 757 \text{ kJ/mol}$  un homeostāzes Lehningera  $G_{\text{C}_6\text{H}_{12}\text{O}_6} = 2268,8 \text{ kJ/mol}$ . [8,6]

Ģenerētie  $6\text{HCO}_3^- + 6\text{H}_3\text{O}^+$  joni virza  $6\text{O}_2\text{aqua} + 6\text{H}_2\text{O}$  cauri membrānu akvaporīnu kanāliem osmozē pretēji koncentrācijas gradientiem, bet transportē jonus  $6\text{HCO}_3^- + 6\text{H}_3\text{O}^+$  lejup pa gradientiem cauri membrānu bikarbonāta un protonu kanāliem lietojot homeostāzes producēto  $\Delta G_{\text{Lehninger}} = -2840 \text{ kJ/mol}$  brīvo enerģiju.



Potenciālu starpība  $\Delta E = \Delta G_{eq} / F \cdot n = (E^\circ_{C_6H_{12}O_6} - E^\circ_{O_2}) = -2840000 / 96485 / 24 = -1,2264$  V dod **absolūto** standarta potenciālu  $E^\circ_{C_6H_{12}O_6} = \Delta E + E_{O_2} = -1,226 + 1,0868 = -0,1392$  V glikozes pusreakcijai no Lehningera **-2840** kJ/mol. [6]

Nernsta pus reakcijai  $C_6H_{12}O_6 + 42H_2O = 30H_3O^+ + 6HCO_3^- + 24e^-$  ir standarta potenciāls  $E^\circ_{C_6H_{12}O_6} = -0,1392$  V : Alberty dati sakrīt ar **absolūto** potenciālu skalu. Skābekļa reducēšanas  $O_{2(aqua)} + 4H_3O^+ + 4e^- = 6H_2O$  **inversais** standarta potenciāls  $-E^\circ_{O_2} = -1,0868$  V ir **inverss**, jo produkti ir ūdens molekulas nevis skābeklis:

$$\Delta G_{O_{2(aq)}Alberty} = 6G_{H_2O} - (G_{O_{2(aq)}} + 4G_{H_3O^+}) = 6 \cdot 0 - (330,4 \cdot 22,44) = -419,76 \text{ kJ/mol:}$$

**Absolūtās** enerģijas izmaiņas minimums  $\Delta G_{eqStandardO_2} = -E^\circ_{O_2} \cdot F \cdot 1 \cdot 4 = -1,0868 \cdot 96485 \cdot 4 = -419,44$  kJ/mol ar sešām skābekļa molekulu pus reakcijām oksidē glikozi (**Glc**) atbrīvojot enerģiju izmaiņā  $\Delta G_{Homeostāzes} = -2840$  kJ/mol.

Standarts  $\Delta G_{AlbertyAbsoluteC_6H_{12}O_6} = E^\circ_{C_6H_{12}O_6} \cdot F \cdot 1 \cdot 24 = -0,1392 \cdot 96485 \cdot 24 = -322$  kJ/mol ir eksoerģiska **absolūtās** brīvās enerģijas izmaiņa. Pus reakciju summa parāda sakrītību Alberty datiem ar **absolūto** potenciālu skalu:

$$6\Delta G_{eqStandardO_2} = 6 \cdot -419,44 = -2516,6 \text{ kJ/mol} ; 6\Delta G_{O_{2(aq)}Alberty} = 6 \cdot -419,76 = -2518,6 \text{ kJ/mol};$$

$$6\Delta G_{eqStandardO_2} + \Delta G_{AlbertyAbsoluteC_6H_{12}O_6} = -2516,6 - 322 = -2838,94 \text{ kJ/mol} ;$$

**Inversie** standarta potenciāli  $-E^\circ_{O_2} = -1,0868$  V ar homeostāzes atraktoriem  $[H_3O^+] = 10^{-(7,36)}$  M,  $[HCO_3^-] = 0,0154$  M,  $[C_6H_{12}O_6] = 5 \cdot 10^{-(3)}$  M,  $[O_{2(aqua)}] = 6 \cdot 10^{-5}$  M,  $[H_2O] = 55,3$  M rada **absolūto** potenciālu summu skābeklim un glikozei eksoerģiskāku  $\Delta G_{Lehninger} = -2840$  kJ/mol  $<$   $\Delta G_{Homeostāze} = -3054,7$  kJ/mol :

$$E_{O_2} = -E^\circ_{O_2} + \frac{0,0591}{4} \cdot \log\left(\frac{[H_2O]^6}{[O_{2(aqua)}][H_3O^+]^4}\right) = -1,0868 + \frac{0,0591}{4} \cdot \log\left(\frac{55,346^6 / 6 / 10^{-(5)}}{10^{-(7,36 \cdot 4)}}\right) = -0,4349 \text{ V}$$

$$\text{un: } E_{C_6H_{12}O_6} = E^\circ_{C_6H_{12}O_6} + \frac{0,0591}{24} \cdot \log\left(\frac{[HCO_3^-]^6 \cdot [H_3O^+]^{30}}{[C_6H_{12}O_6][H_2O]^{42}}\right) =$$

$$= -0,1392 + \frac{0,0591}{24} \cdot \log\left(\frac{0,0154^6 \cdot 10^{-(7,36 \cdot 30)}}{5 / 10^{-(3)} / 55,346^{42}}\right) = -0,8843 \text{ Volti .}$$

Brīvā enerģijas izmaiņa ir eksoerģiska, negatīva vērtība standarta un homeostāzes apstākļos:

$$\Delta G_{Lehninger} = \Delta E \cdot F \cdot n = (E^\circ_{C_6H_{12}O_6} - E^\circ_{O_2}) \cdot F \cdot n = (-0,1392 - 1,0868) \cdot F \cdot n = -1,226 \cdot 96485 \cdot 24 = -2840 \text{ kJ/mol.}$$

$$\Delta G_{Homeostāzes} = \Delta E \cdot F \cdot n = (E^\circ_{C_6H_{12}O_6} - E^\circ_{O_2}) \cdot F \cdot n = (-0,88427 - 0,4349) \cdot F \cdot n = -1,31917 \cdot 96485 \cdot 24 = -3054,7 \text{ kJ/mol.}$$

Skābekļa reducēšanas  $6(O_{2(aqua)} + 4H_3O^+ + 4e^- \rightleftharpoons 6H_2O)$ ; **inversais** standarta potenciāls  $E^\circ_{O_2} = 1,0868$  Volti un glikozes homeostāzes konstante ar atraktoriem  $[H_3O^+] = 10^{-7,36}$  M,  $[HCO_3^-] = 0,0154$  M,  $[C_6H_{12}O_6] = 5 \cdot 10^{-3}$  M, ūdeni  $[H_2O] = 55,3$  M un  $\Delta G_{Lehninger} = -2840$  kJ/mol ir lielāka par vienu  $K_{eqHomeostāzes} = 10^{498}$ :

$$K_{eqHomeostāzes} = \frac{[HCO_3^-]^6 [H_3O^+]^6}{[C_6H_{12}O_6] \cdot [O_2]^6 [H_2O]^6} = \text{EXP}(-\Delta G_{eqHomeostāzes} / R / T) = \text{EXP}(2840000 / 8,3144 / 298,15) = 10^{498}:$$

Kvazi līdzsvara stāvoklis virzīts neatgriezeniskā sintēzē, kura kā dzinējs akumulē brīvo enerģiju produktos:



$$\text{Hesa likumā } 2840 \text{ kJ/mol} = G_{C_6H_{12}O_6} + 6 \cdot G_{O_2Homeostāzes\_arterial} + 6 \cdot G_{H_2O\_Biochem} - (6 \cdot G_{H_3O^+} + 6 \cdot G_{HCO_3^-})$$

brīvās enerģijas saturs vienā molā glikozes ir aprēķināts atsaucoties uz Alberty datiem. [8,15]

Veidošanās no elementiem  $S_{\text{rombisks}} + H_2\text{gāze} = H_2S_{\text{gāze}}$ ;  $G_{S_{\text{rombisks}}} = -85,64 \text{ kJ/mol}$ ; [1,6]

Veidošanās enerģijas izmaiņa ir  $\Delta G_{\text{Hess}, H_2S_{\text{gāze}}} = G^\circ_{H_2S_{\text{gāze}}} - (G_{\text{rombisks}} + G_{H_2}) = -20,6 - (0 + 0) = -20,6 \text{ kJ/mol}$ .

Sēra enerģijas saturs molā ir  $G_{S_{\text{rombisks}}} = G^\circ_{H_2S_{\text{gāze}}} - (\Delta G_{\text{Hess}, H_2S_{\text{gāze}}} + G^\circ_{H_2\text{gāze}}) = -20,6 - (-20,6 + 85,64) = -85,64 \text{ kJ/mol}$ ;

Brīvās enerģijas saturs sērūdeņraža šķīdumā  $G_{H_2S_{\text{aqua}}} = -30,82 \text{ kJ/mol}$ . [1,6]

Sēra reducēšanas Nernsta pus reakcijai  $H_2S_{\text{aq}} + 2H_2O = S_{\text{rombisks}} + 2H_3O^+ + 2e^-$  ir absolūtais standarta potenciāls  $E^\circ_{H_2S} = -0,0515 \text{ V}$  brīvās enerģijas izmaiņai  $\Delta G_{\text{eq}, H_2S} = E^\circ_{H_2S} F n = -0,0515 * 96485 * 2 = -9,938 \text{ kJ/mol}$ . Tā uzrāda brīvās enerģijas saturu vienā molā  $G_{H_2S_{\text{aqua}}} = -30,82 \text{ kJ/mol}$ , kā izteiksme no Hesa likuma brīvās enerģijas izmaiņai pus reakcijā  $\Delta G_{\text{Hess}, H_2S_{\text{aq}}} = G_{S_{\text{rombisks}}} + 2G_{H_3O^+} - (G_{H_2S_{\text{aq}}} + 2G_{H_2O}) = -85,64 + 2 * 22,44 - (G_{H_2S_{\text{aq}}} + 2 * 0) = -9,938 \text{ kJ/mol}$  sērūdeņraža ūdens šķīdumā:

$$G_{H_2S_{\text{aq}}} = G_{S_{\text{rombisks}}} + 2G_{H_3O^+} - (\Delta G_{\text{Hess}, H_2S_{\text{aq}}} + 2G_{H_2O}) = -85,64 + 2 * 22,44 - (-9,938 + 2 * 0) = -30,82 \text{ kJ/mol}$$

Sēra **inversā** pus reakcija  $S_{\text{rombisks}} + 2H_3O^+ + 2e^- = H_2S_{\text{aq}} + 2H_2O$ ;  $-E^\circ_{H_2S} = 0,0515 \text{ Volti}$  ar diviem metāla ūdeņraža moliem pus reakcijā  $2(\text{Pt})H + 2H_2O \leftrightarrow 2H_3O^+ + 4e^-$ ;  $E^\circ_H = -0,2965 \text{ V}$  absolūtā standart potenciālu summa ir:

$$\Delta E^\circ_{\text{Red-Ox}} = (E^\circ_H - E^\circ_{H_2S}) = (-0,2965 + 0,0515) = -0,245 \text{ Volti}$$

Metāls ūdeņradis  $(\text{Pt})H$  reducē rombisko sēru:  $S_{\text{rombisks}} + 2(\text{Pt})H = H_2S_{\text{aq}}$ ; par ūdeņraža sulfīdu.

Brīvās enerģijas izmaiņas minimums metāla ūdeņraža  $(\text{Pt})H$  oksidēšanas ar sēru līdzsvara stāvoklī: ir negatīvs:

$$\Delta G_{\text{eq}} = (E^\circ_H - E^\circ_{H_2S}) \cdot F \cdot 1 \cdot 2 = (-0,2965 + 0,0515) * 96485 * 2 = -0,245 * 96485 * 2 / 1000 = -47,28 \text{ kJ/mol}$$
; [CRC](#) [1]

Brīvās enerģijas izmaiņas izteiksme no Hesa likuma:

$$\Delta G_{\text{Hess}, H_2S} = G_{H_2S_{\text{aqua}}} - (2G_{H(\text{Pt})} + G_{S_{\text{rombisks}}}) = G_{H_2S_{\text{aqua}}} - (2 * 51,05 - 85,64) = -47,28 \text{ kJ/mol}$$
 uzrāda

sērūdeņraža šķīdumā identisku negatīvu enerģijas saturu kā  $G_{H_2S_{\text{aqua}}} = -30,82 \text{ kJ/mol}$  reducēšanas pusreakcijā atsevišķi:

$$G_{H_2S_{\text{aqua}}} = \Delta G_{\text{Hess}, H_2S} + (2G_{H(\text{Pt})} + G_{S_{\text{rombisks}}}) = -47,28 + (2 * 51,05 - 85,64) = -30,82 \text{ kJ/mol}$$

Alberty dati sakrīt ar absolūto standarta potenciālu skalu abās pusreakcijās kā atsevišķā  $E^\circ_{H_2S} = -0,0515 \text{ V}$  un tā arī sasaistītajās nokomplektētajās oksidēšanas - reducēšanas reakcijās ar standard potential summu līdzīgi kā

$$\Delta E^\circ_{\text{Red-Ox}} = (E^\circ_H - E^\circ_{H_2S}) = (-0,2965 + 0,0515) = -0,245 \text{ Volts}$$

Ūdeņraža elektroda atskaites noteikšana  $E^\circ_H = -0,2965 \text{ Volti}$  **absolūtā potenciāla skalā** sinhronizē zinātnes ar **absolūto** brīvās enerģijas skalas mērogu.

Ūdeņraža elektroda atskaites punkta  $E^\circ_H = -0,2965 \text{ V}$  atklāšana **absolūtajam** potenciālam un **absolūtās** brīvās enerģijas skalai ar inversās simetrijas nozīmi pusreakcijā, kurai **inversais** potenciāls piemīt viens un tas pats skaitlis ar pretēju zīmi, jo simetrija sakrīt ar **inverso** absolūto brīvo enerģiju, tas pats skaitlis ar pretēju zīmi.

**Absolūtās** un **inversās** brīvās enerģijas un potenciāla mēroga noteikšanai ir nepieciešama ūdens un hidroksonija uzskaitē, pamatojoties uz Alberty datiem par ūdeņraža gāzes un šķīduma termodinamisko **absolūto** brīvo enerģiju.

**Absolute** Free Energy scale requires applied zero to water and carbon dioxide gas background reference for metabolites shown in Figure 1..

**Absolūtās** brīvās enerģijas skalai ir jāpiemēro metabolītu nulles vērtība ūdenim un oglekļa dioksīda gāzes fona atsauce, kas parādīti 1. attēlā.

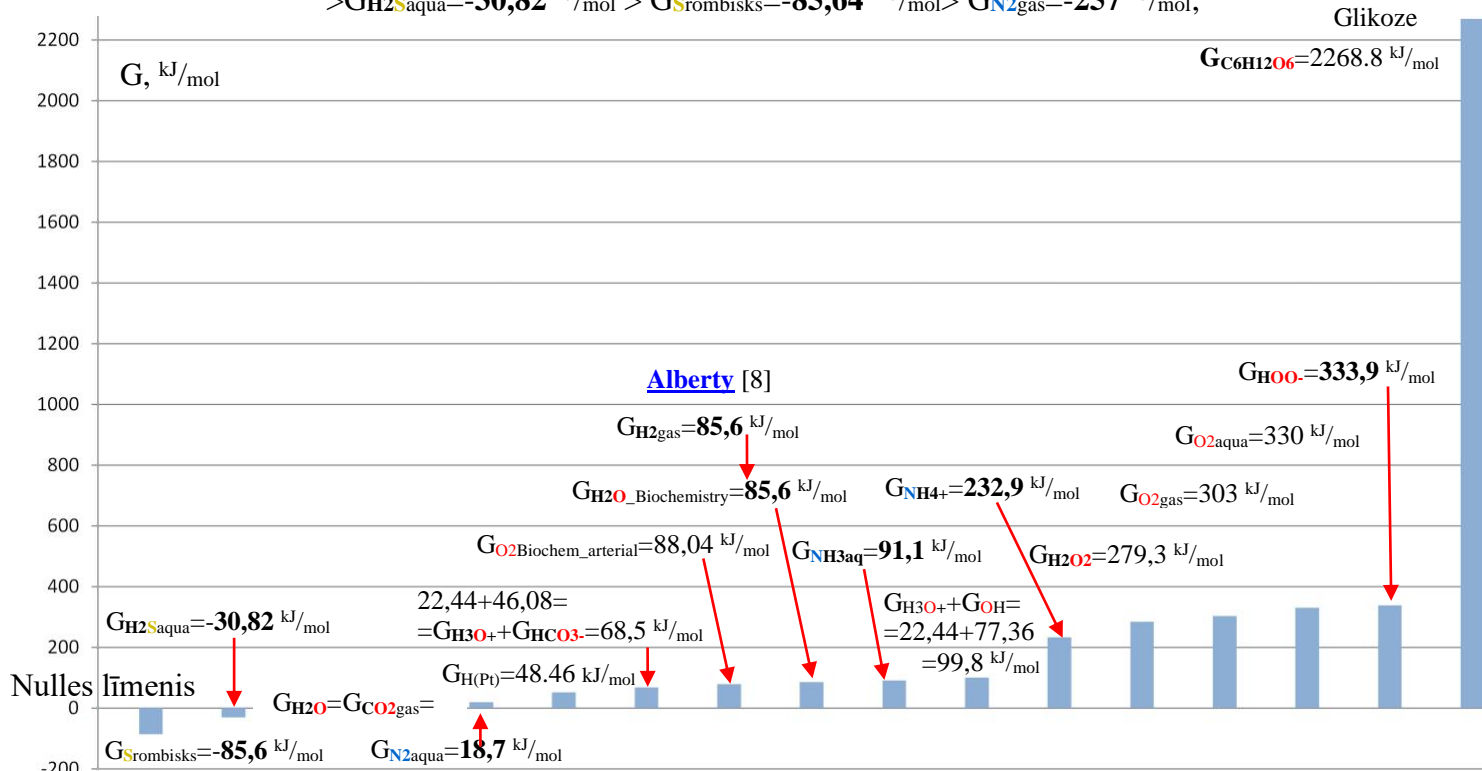
**Inversijas** simetrija, ko abpusējas atbilstības rezultātā izmanto kā termodinamiskos rīkus: **absolūtās** brīvās enerģijas un **absolūto potenciālu skalu**, lai atklātu Nernsta pus-, **inverso**- un pilno oksidēšanas-reducēšanas reakciju strukturālās detaļas.

Hesa elementu nulles standarta vērtības patiesībā ir pozitīvas bioķīmijas enerģijas.

$G_{H_2gas} = -85,6 \text{ kJ/mol}$  [Alberty](#) attiecinātas uz homeostāzes productu ūdens un  $CO_2gas$  nulli  $G_{H_2O} = G_{CO_2gas} = 0 \text{ kJ/mol}$ .

Dažu [reaktantu](#) [1,8] brīvās enerģijas saturs attiecināti uz homeostāzes produktu nulles vērtību skalu ir:

Glikoze  $G_{C_6H_{12}O_6} = 2268,8 \text{ kJ/mol} >$  deprotonēts peroksīda anjons  $G_{HO_2} = 338 \text{ kJ/mol} >$   $G_{O_2aqua} = 330 \text{ kJ/mol} >$   
 $>$   $G_{O_2gas} = 303 \text{ kJ/mol} >$  peroksīds  $G_{H_2O_2} = 284 \text{ kJ/mol} >$   $G_{NH_4^+} = 232,9 \text{ kJ/mol} >$   
 $>$  ūdens protolīzes  $pH = pOH = 7$   $G_{H_3O^+ + OH^-} = G_{H_3O^+} + G_{OH^-} = 22,44 + 77,36 = 99,8 \text{ kJ/mol} >$   
 $>$   $G_{NH_3aq} = 91,1 \text{ kJ/mol} >$   $G_{H_2gas} = -85,6 \text{ kJ/mol} \equiv G_{H_2O\_Biochemistry} = -85,6 \text{ kJ/mol} >$   $G_{O_2Biochem\_arterial} = 78,1 \text{ kJ/mol} >$   
 $>$   $CO_2aqua$  šķīduma protolīze ar karbo anhidrāzi  $G_{H_3O^+ + HCO_3^-} = G_{H_3O^+} + G_{HCO_3^-} = 22,44 + 46,08 = 68,5 \text{ kJ/mol} >$   
 $>$   $G_{H(Pt)} = 51 \text{ kJ/mol} >$  homeostāzes produktu nulles vērtības  $G_{H_2O} = G_{CO_2gas} = 0 \text{ kJ/mol} >$   
 $>$   $G_{H_2S_{aqua}} = -30,82 \text{ kJ/mol} >$   $G_{S_{rombisks}} = -85,64 \text{ kJ/mol} >$   $G_{N_2gas} = -257 \text{ kJ/mol};$



Grafiks 1. Augoša **absolūtās** brīvā enerģija metabolītiem attiecināta uz  $G_{H_2O} = G_{CO_2gas} = 0 \text{ kJ/mol}$  nulles vērtību.

Atklājums zinātnē par **Absolūto potenciālu skalu** ir sakrītošs ar **absolūtās** brīvās enerģijas nozīmīgi.

Ūdens un hidroksionija atlaide reakcijās ieskaitot protolīzi un elektroķīmiju Nernsta pus reakcijās ierobežo zinātniskās studijas termodinamikā, fizikālā ķīmijā un bioķīmijā. [8,14,15]

**Inversijas simetrijas** termodinamiskā īpašība ir tieša reakcija starp reaģentiem un produktiem, kas apgriežas pretējā virzienā, sākotnēji nozīmējot produktus kā reaģentus un atstājot reaģentus kā galaproduktus. Ūdeni par skābekli oksidēšanas reducēšanas  $6H_2O = O_{2aqua} + 4H_3O^+ + 4e^-$  Nernsta pus reakcijā ir **absolūtais standarta potenciāls**:  $E^{\circ}_{O_2Absolute} = 1.0868 \text{ V}$ . Par  $O_{2aqua} + 4H_3O^+ + 4e^- = 6H_2O$  iesaistīšanos **inversajā** reakcijā **absolūtam potenciālam** ir vienāds skaitlis ar pretēju zīmi  $E^{\circ}_{O_2Absolute} = -1.0868 \text{ V}$  negatīvs.

Atklātā **absolūtā potenciāla skala** Nernsta vai **inversajām** reakcijām sakrīt ar **absolūtās** brīvās enerģijas īpašību **inversajā simetrijā**. [8, 14, 15] Nernsta vai **inverso** reakciju **inversās simetrijas** īpašība ar identiskām vērtībām, bet ar **pretēju zīmi**, kas izpaužas **absolūtā potenciāla skalā** ar **absolūto** brīvo enerģiju, ir sakrītīga termodinamiskā īpašība protolīzes reakcijai, Nernsta pusreakcijai vai **inversajai** reakcijai.

Koriģētā metāla ūdeņraža termodinamiskā standarta potenciāla atskaite 0,10166 Volti dažu gadu laikā dod impulsu zinātnēm iegūt **absolūtās** termodinamiskās vērtības elementu un molekulu brīvajai enerģijai. Pateicoties Alberty dotajiem datiem par ūdeņraža **absolūto** brīvo enerģiju gāzei  $G_{H_2gas} = -85.6 \text{ kJ/mol}$  un  $G_{H_2aqua} = -103 \text{ kJ/mol}$  šķīdumā ir noteikti **absolūtie** standarta potenciāli metāla ūdeņraža vispārīgā atskaite  $E^{\circ}_{H} = -0.2965 \text{ Voltos}$ . Tabulā 1. tiek publicētas 50 bioķīmijā lietotas Nernsta oksidēšanas pus vai reducēšanas **inversās** reakcijas.

Trijos stabiņos mēs varam novērot attīstību ūdeņraža vispārīgai atskaites skalai no klasiskās nulles  $E^{\circ}_{H} = 0 \text{ V}$  ar ūdens atlaidi. Ūdens un hidroksionija katjona uzskaitē koriģē vispārīgo ūdeņraža termodinamisko standarta skalas atskaites potenciālu uz  $E^{\circ}_{H} = 0.10166 \text{ Voltiem}$ . Trešajā stabiņā Alberty dati beidzot noved pie **absolūtās** standarta **potenciāla** vērtības  $E^{\circ}_{H} = -0.29654 \text{ Volti}$  ūdeņraža elektrodam.

**H<sub>2</sub>O<sub>2</sub> veidošanās** 41. lapa  $\text{H}_{2\text{gas}} + \text{O}_{2\text{gas}} \Rightarrow \text{H}_2\text{O}_2$ ;  $\Delta G^\circ_{\text{UnivAlberta}} = -134,03 \text{ kJ/mol}$ ;  $\Delta G^\circ_{\text{Alberty}} = -48,39 \text{ kJ/mol}$ ;

$$\Delta G_{\text{Alberty}} = G_{\text{H}_2\text{O}_2} - (G_{\text{O}_2\text{gas}} + G_{\text{H}_2\text{gas}}) = \underline{284,25} - (85,64 + 303) = -104,64 \text{ kJ/mol} (-134,03 \text{ kJ/mol};) (= -48,39 \text{ kJ/mol})$$

Viela	$\Delta H^\circ_{\text{H}} \text{ kJ/mol}$	$\Delta S^\circ_{\text{H}} \text{ J/mol/K}$	$\Delta G^\circ_{\text{H}} \text{ kJ/mol}$
<b>H<sub>2</sub>O<sub>2</sub><sub>aqua</sub></b>	<b>-191,99</b>	<b>-481,688</b>	<b>-48,39</b>
H <sub>2</sub> O <sub>2</sub> <sub>aqua</sub>	-191,17	143,9	-134,03
<b>Succinat<sup>2-</sup></b>	<b>-908,69</b>	<b>-1295,576</b>	<b>-522,414</b>
<b>Fumarate<sup>2-</sup></b>	<b>-776,56</b>	<b>-862,288</b>	<b>-519,4688</b>

Alberty nulles  $G_{\text{H}_2\text{O}} = 0 \text{ kJ/mol}$ ; atskaitē bāzēti  $G_{\text{H}_2\text{O}_2} = \underline{284,25} \text{ kJ/mol}$   
University Alberta

$G_{\text{SuccinatFor}} = -522,4 + (4 \cdot 91,26 + 2 \cdot 85,6 + 2 \cdot 303) = \underline{619,8} \text{ kJ/mol}$ ;  $G_{\text{Succinat}} = \underline{650,8} \text{ kJ/mol}$ ;  
 $G_{\text{FumaricFor}} = -519,5 + (4 \cdot 91,26 + 85,6 + 2 \cdot 303) = \underline{537,1} \text{ kJ/mol}$ ;  $G_{\text{Fumarat}} = \underline{554,75} \text{ kJ/mol}$ ;

**Succinat<sup>2-</sup>** veidošanās  $4\text{C} + 2\text{H}_{2\text{gas}} + 2\text{O}_{2\text{gas}} \Rightarrow (\text{CH}_2)_2(\text{CO}_2^-)(\text{CO}_2^-)$ ;  $\Delta G_{\text{Succinat}} = -522,4 \text{ kJ/mol}$  Alberty;

$$\Delta G_{\text{SuccinatFor}} = G_{\text{SuccinatFor}} - (4G_{\text{Cgraph}} + 2 \cdot G_{\text{H}_2\text{gas}} + 2 \cdot G_{\text{O}_2\text{gas}}) = -522,4 \text{ kJ/mol};$$

$$G_{\text{SuccinatFor}} = -522,4 + (4 \cdot 91,26 + 2 \cdot 85,6 + 2 \cdot 303) = \underline{619,8} \text{ kJ/mol};$$

**Fumarate<sup>2-</sup>** veidošanās  $4\text{C} + \text{H}_{2\text{gas}} + 2\text{O}_{2\text{gas}} \Rightarrow (\text{CH})_2(\text{CO}_2^-)(\text{CO}_2^-)$ ;  $\Delta G_{\text{Fumarat}} = -519,5 \text{ kJ/mol}$  Alberty;

$$\Delta G_{\text{Fumarat}} = G_{\text{FumaratFor}} - (4G_{\text{Cgraph}} + G_{\text{H}_2\text{gas}} + 2 \cdot G_{\text{O}_2\text{gas}}) = -519,5 \text{ kJ/mol};$$

$$G_{\text{FumaratFor}} = -519,5 + (4 \cdot 91,26 + 85,6 + 2 \cdot 303) = \underline{537,1} \text{ kJ/mol}; ; \text{ [veidošanās](#) 73. lapa}$$

**Inversais O<sub>2</sub><sub>aqua</sub> + 2H<sub>3</sub>O<sup>+</sup> + 2e<sup>-</sup> = H<sub>2</sub>O<sub>2</sub><sub>aqua</sub> + 2H<sub>2</sub>O**; standarta potenciāls  $E^\circ_{\text{OxO}_2\text{H}_2\text{O}_2} = -0,5278\text{V}$  University Alberta ;

$$\Delta G_{\text{AlbertyOxO}_2\text{H}_2\text{O}_2} = G_{\text{H}_2\text{O}_2} + 2 \cdot G_{\text{H}_2\text{O}} - (G_{\text{O}_2\text{aqua}} + 2 \cdot G_{\text{H}_3\text{O}^+}) = \underline{279,29} + 2 \cdot 0 - (330 + 2 \cdot 22,44) = -95,59 \text{ kJ/mol};$$

$$\Delta G_{\text{eqAlbertyAbsoluteOxO}_2\text{H}_2\text{O}_2} = E^\circ_{\text{eqOxO}_2\text{H}_2\text{O}_2} \cdot F \cdot 1 \cdot 2 = -0,5278 \cdot 96485 \cdot 2 = -101,85 \text{ kJ/mol};$$

**Succinat<sup>2-</sup> + O<sub>2</sub><sub>aqua</sub> = fumarate<sup>2-</sup> + H<sub>2</sub>O<sub>2</sub><sub>aqua</sub> + Q + ΔG**;  $\Delta G_{\text{min}} = \Delta G_{\text{eqSuccinat\_H}_2\text{O}_2} = -38,3 \text{ kJ/mol}$ ;

$$\Delta G_{\text{Hess}} = \Delta G^\circ_{\text{H}_2\text{O}_2} + \Delta G^\circ_{\text{fumarat}} - \Delta G^\circ_{\text{O}_2} - \Delta G^\circ_{\text{Succinat}} = -48,39 - 519,4688 - (16,4 - 522,414) = -61,845 \text{ kJ/mol};$$

$$\Delta G_{\text{min}} = \Delta G_{\text{eq}} = (E^\circ_{\text{RedSuccinate}} - E^\circ_{\text{OxO}_2}) \cdot F \cdot n = (0,2512 - 0,4495) \cdot 96485 \cdot 2 = (-0,1983) \cdot 96485 \cdot 2 = -38,3 \text{ kJ/mol};$$

$$\text{Alberty Hesa } \Delta G_{\text{Succinat\_H}_2\text{O}_2} = G_{\text{Fumarat}} + G_{\text{H}_2\text{O}_2} - (G_{\text{Succinat}} + G_{\text{O}_2\text{aqua}}) = 537,1 + 284,24 - (619,8 + 330) = -128,5 \text{ kJ/mol};$$

$$K_{\text{eq}} = \exp(-\Delta G_{\text{eq}}/R/T) = \exp(38270/8,3144/298,15) = 5065991 \text{ [veidošanās](#) 58. Lapa.}$$

**Absolūto** termodinamisko parametru jēdzieni temperatūra, brīvā enerģija un potenciāls ir **absolūti** savstarpēji instrumenti, lai atklātu paralēlu un secīgu komplekso reakciju strukturālās detaļas, izmantojot inversijas simetrijas īpašības.

1. **Absolūtā** temperatūra T Kelvina grādos ir standarta vērtībā 298.15 K (25 ° C),

Lord Kelvin



2. Uz Alberty bāzētais absolūtais brīvās enerģijas saturs

$G_{\text{H}_2\text{gas}} = 85,6 \text{ kJ/mol}$  ūdeņraža gāzei, tās šķīdumam ūdenī  $G_{\text{H}_2\text{aqua}} = 103 \text{ kJ/mol}$  un

[metālam](#) ūdeņradim  $G_{\text{H(Pt)}} = 48,46 \text{ kJ/mol}$

atsaucoties uz nulles atskaites vērtību  $G_{\text{H}_2\text{O}} = G_{\text{CO}_2\text{gas}} = 0 \text{ kJ/mol}$  kā fonu

ūdenī un oglekļa dioksīda gāzē  $\text{CO}_{2\text{gas}}$ .

Alberty Robert



3. Atklājums **Absolūtā potenciālu** skala.

**Absolūtā potenciāla** skala, pamatojas uz vispārīgu atsauci metāla ūdeņraža absolūto standarta Potenciālu  $E^\circ_{\text{H}} = -0.2965 \text{ Volti}$ . [8, 14, 15]



**CH<sub>3</sub>CH<sub>2</sub>OH** etanola veidošanās no elementiem:

$$2\text{C}+3\text{H}_{2\text{gas}}+1/2\text{O}_{2\text{gas}}=>\text{CH}_3\text{CH}_2\text{OH}; \Delta G^\circ_{\text{Alberty}}=75,2864 \text{ kJ/mol}; \Delta G^\circ_{\text{HessCRC}}=-181 \text{ kJ/mol};$$

$$\Delta G^\circ_{\text{Alberty}}=G_{\text{CH}_3\text{CH}_2\text{OH}}-(2G_{\text{Cgraph}}+3G_{\text{H}_2\text{gas}}+1/2G_{\text{O}_2\text{gas}})=75,2864 \text{ kJ/mol};$$

$$\Delta G^\circ_{\text{CRC}}=G_{\text{CH}_3\text{CH}_2\text{OH}}-(2G_{\text{Cgraph}}+3G_{\text{H}_2\text{gas}}+1/2G_{\text{O}_2\text{gas}})=-181 \text{ kJ/mol};$$

$$\Delta G^\circ_{\text{Alberty}}+(2G_{\text{Cgraph}}+3G_{\text{H}_2\text{gas}}+1/2G_{\text{O}_2\text{gas}})=75,2864+(2*91,26+3*85,6+1/2*303)=G_{\text{CH}_3\text{CH}_2\text{OH}}=666,106 \text{ kJ/mol};$$

$$\Delta G^\circ_{\text{CRC}}+(2G_{\text{Cgraph}}+3G_{\text{H}_2\text{gas}}+1/2G_{\text{O}_2\text{gas}})=-181+(2*91,26+3*85,6+1/2*303)=G_{\text{CH}_3\text{CH}_2\text{OH}}=409,82 \text{ kJ/mol};$$

**CH<sub>3</sub>CHO** acetaldehīda veidošanās no elementiem:  $2\text{C}+2\text{H}_{2\text{gas}}+1/2\text{O}_{2\text{gas}}=>\text{CH}_3\text{CHO}$ ;

$$\Delta G^\circ_{\text{Alberty}}=G_{\text{CH}_3\text{CHO}}-(2G_{\text{Cgraph}}+2G_{\text{H}_2\text{gas}}+1/2G_{\text{O}_2\text{gas}})=32,282 \text{ kJ/mol};$$

$$\Delta G^\circ_{\text{CRC}}=G_{\text{CH}_3\text{CHO}}-(2G_{\text{Cgraph}}+2G_{\text{H}_2\text{gas}}+1/2G_{\text{O}_2\text{gas}})=24,06 \text{ kJ/mol};$$

$$\Delta G^\circ_{\text{Alberty}}+(2G_{\text{Cgraph}}+2G_{\text{H}_2\text{gas}}+1/2G_{\text{O}_2\text{gas}})=32,282+(2*91,26+2*85,6+1/2*303)=G_{\text{CH}_3\text{CHO}}=537,5 \text{ kJ/mol};$$

$$\Delta G^\circ_{\text{CRC}}+(2G_{\text{Cgraph}}+2G_{\text{H}_2\text{gas}}+1/2G_{\text{O}_2\text{gas}})=24,06+(2*91,26+2*85,6+1/2*303)=G_{\text{CH}_3\text{CHO}}=529,28 \text{ kJ/mol};$$

$$\text{CH}_3\text{CH}_2\text{OH}+\text{H}_2\text{O}=\text{CH}_3\text{CHO}+\text{H}_3\text{O}^++\text{H}^+(\text{H}^++2\text{e}^-); \text{absolūtais potenciāls } E^\circ_{\text{CH}_3\text{CH}_2\text{OH}}=-0,055 \text{ V}; [19]$$

$$\Delta G_{\text{eqCH}_3\text{CH}_2\text{OH}}=E^\circ_{\text{eqNernsCH}_3\text{CH}_2\text{OH}}*F*2=-0,055*96485*2=-10,6 \text{ kJ/mol};$$

$$\Delta G_{\text{HessCH}_3\text{CH}_2\text{OH}}=G_{\text{CH}_3\text{CHO}}+G_{\text{H}_3\text{O}^+}+G_{\text{H}^-}-(G_{\text{CH}_3\text{CH}_2\text{OH}}+G_{\text{H}_2\text{O}})=537,5+22,44+G_{\text{H}^-}-(409,82+0)=-10,6 \text{ kJ/mol}.$$

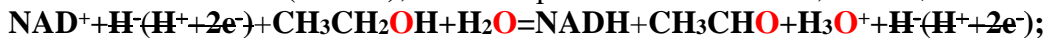
$$\Delta G_{\text{HessCH}_3\text{CH}_2\text{OH}}=G_{\text{CH}_3\text{CHO}}+G_{\text{H}_3\text{O}^+}+G_{\text{H}^-}-(G_{\text{CH}_3\text{CH}_2\text{OH}}+G_{\text{H}_2\text{O}_{\text{Biochem}}})=537,5+22,44+G_{\text{H}^-}-(409,82+85,64)=-10,6 \text{ kJ/mol}.$$

$$\Delta G_{\text{HessCH}_3\text{CH}_2\text{OH}}-G_{\text{CH}_3\text{CHO}}-G_{\text{H}_3\text{O}^+}+(G_{\text{CH}_3\text{CH}_2\text{OH}}+G_{\text{H}_2\text{O}})=G_{\text{H}^-}=-10,6-537,5-22,44+(409,82+0)=-160,7 \text{ kJ/mol}.$$

$$\Delta G_{\text{HessCH}_3\text{CH}_2\text{OH}}-G_{\text{CH}_3\text{CHO}}-G_{\text{H}_3\text{O}^+}+(G_{\text{CH}_3\text{CH}_2\text{OH}}+G_{\text{H}_2\text{O}_{\text{Biochem}}})=G_{\text{H}^-}=-10,6-537,5-22,44+(409,82+85,64)=-75,08 \text{ kJ/mol}.$$

Viela	$\Delta H^\circ_{\text{H}} \text{ kJ/mol}$	$\Delta S^\circ_{\text{H}} \text{ J/mol/K}$	$\Delta G^\circ_{\text{H}} \text{ kJ/mol}$	CRC Handbook of Chemistry and Physics 2010 90th David R. Lide
<b>H<sub>3</sub>C-CH=O</b>	-212,23	-281,84	24,06	$G_{\text{CH}_3\text{CHO}}=529,28 \text{ kJ/mol};$
<b>H<sub>3</sub>C-CH=O</b>	<b>-213,88</b>	<b>-825,64</b>	<b>32,2824</b>	$G_{\text{CH}_3\text{CHO}}=537,5 \text{ kJ/mol};$
NADH	-41,41	-4465,708	1175,5732	BioThermodynam06;
NADH	-1036,66	-140,50	1120,09	
<b>H<sub>3</sub>O<sup>+</sup></b>	-285,81	-3,854	-213,275	
NAD <sup>+</sup>	<b>-10,30</b>	<b>-3766,008</b>	<b>1112,534</b>	BioThermodynamic,2006,Massachusetts Tecnology Institute,Alberty
NAD <sup>+</sup>	-1007,48	-183	1059,11	
<b>H<sub>3</sub>CCH<sub>2</sub>OH</b>	<b>-290,77</b>	<b>-1227,764</b>	<b>75,2864</b>	Alberty $G_{\text{CH}_3\text{CH}_2\text{OH}}=666,106 \text{ kJ/mol};$
H <sub>3</sub> CCH <sub>2</sub> OH <sub>aq</sub>	-288,3	-357,7394	-181,64	CRC $G_{\text{CH}_3\text{CH}_2\text{OH}}=409,82 \text{ kJ/mol};$
<b>H<sub>2</sub>O</b>	-285,85	69,9565	-237,191	$G_{\text{H}_2\text{O}}=0 \text{ kJ/mol}; G_{\text{H}^-}=-10,6-537,5-22,44+(409,82+0)=-160,7 \text{ kJ/mol}.$
<b>H<sub>2</sub>O</b>	<b>-286,65</b>	<b>-453,188</b>	<b>-151,549</b>	$G_{\text{H}_2\text{O}_{\text{Biochem}}}=85,64 \text{ kJ/mol}. G_{\text{H}^-}=-10,6-537,5-22,44+(409,82+85,64)=-75,08 \text{ kJ/mol}$

$\text{NADH} = \text{NAD}^+ + \text{H}^+(\text{H}^++2\text{e}^-)$ ; inversais potenciāls  $-E^\circ_{\text{NADH}}=0,4095 \text{ V}$ ; absolute David Harris; [22]



$$\text{summa: } E^\circ_{\text{eqNernsCH}_3\text{CH}_2\text{OH}}-E^\circ_{\text{NAD}^+}=-0,055+0,4095=0,4562;$$

$$\Delta G_{\text{min}}=\Delta G_{\text{eq}}=(E^\circ_{\text{eqNernsCH}_3\text{CH}_2\text{OH}}-E^\circ_{\text{NAD}^+})*F*n=(-0,055+0,4095)*96485*2=0,4562*96485*2=68,408 \text{ kJ/mol};$$

$$\Delta G_{\text{HessAlbertyCH}_3\text{CH}_2\text{OH}}=G_{\text{NADH}}+G_{\text{H}_3\text{O}^+}+G_{\text{CH}_3\text{CHO}}-(G_{\text{NAD}^+}+G_{\text{CH}_3\text{CH}_2\text{OH}}+G_{\text{H}_2\text{O}})=68,02 \text{ kJ/mol}.$$

$$=1112,534+22,44+32,282-(1175,5+75,2864-151,549)=68,02 \text{ kJ/mol}.$$



$$\Delta G_{\text{eqH}_3\text{CHC}(\text{OH})\text{COO}^-} = E^\circ_{\text{eqH}_3\text{CHC}(\text{OH})\text{COO}^-} \cdot F \cdot 2 = -0,0159 \cdot 96485 \cdot 2 = -3,068 \text{ kJ/mol};$$

$$\Delta G_{\text{HessCH}_3\text{CH}_2\text{OH}} = G_{\text{H}_3\text{CC}=\text{OCOO}^-} + G_{\text{H}_3\text{O}^+} + G_{\text{H}^-} - (G_{\text{H}_3\text{CHC}(\text{OH})\text{COO}^-} + G_{\text{H}_2\text{O}}) = 534,2 + 22,44 + G_{\text{H}^-} - (668,8 + 0) = -3,068 \text{ kJ/mol}.$$

$$\Delta G_{\text{HessCH}_3\text{CH}_2\text{OH}} = G_{\text{H}_3\text{CC}=\text{OCOO}^-} + G_{\text{H}_3\text{O}^+} + G_{\text{H}^-} - (G_{\text{H}_3\text{CHC}(\text{OH})\text{COO}^-} + G_{\text{H}_2\text{O}_{\text{Biochem}}}) = 534,2 + 22,44 + G_{\text{H}^-} - (668,8 + 85,64) = -3,068 \text{ kJ/mol}.$$

$$\Delta G_{\text{HessCH}_3\text{CH}_2\text{OH}} - G_{\text{H}_3\text{CC}=\text{OCOO}^-} - G_{\text{H}_3\text{O}^+} + (G_{\text{H}_3\text{CHC}(\text{OH})\text{COO}^-} + G_{\text{H}_2\text{O}}) = G_{\text{H}^-} = -3,068 - 534,2 - 22,44 + (668,8 + 0) = 109,092 \text{ kJ/mol}.$$

$$\Delta G_{\text{HessCH}_3\text{CH}_2\text{OH}} - G_{\text{H}_3\text{CC}=\text{OCOO}^-} - G_{\text{H}_3\text{O}^+} + (G_{\text{H}_3\text{CHC}(\text{OH})\text{COO}^-} + G_{\text{H}_2\text{O}_{\text{Biochem}}}) = G_{\text{H}^-} = -3,068 - 534,2 - 22,44 + (668,8 + 85,64) = 194,7 \text{ kJ/mol}.$$

$$I = 0,25 \text{ M, BioTherm06, pH} = 7,36, \Delta G_{\text{H}} = G^\circ_{\text{H}_3\text{CC}=\text{OCOO}^-} + G^\circ_{\text{H}_3\text{O}^+} + G_{\text{H}^-} - G_{\text{H}_3\text{CHC}(\text{OH})\text{COO}^-} - G_{\text{H}_2\text{O}} = \text{kJ/mol};$$

$$\text{Viola } \Delta H^\circ_{\text{H}} \text{ kJ/mol } \Delta S^\circ_{\text{H}} \text{ J/mol/K } \Delta G^\circ_{\text{H}} \text{ kJ/mol};$$

<b>PyruvEnolP<sup>3-</sup></b>	-1400	-1100	-1189,73	$G_{\text{H}_2\text{O}} = 0 \text{ kJ/mol}; G_{\text{H}^-} = -3,068 - 534,2 - 22,44 + (668,8 + 0) = 109,092 \text{ kJ/mol}$
<b>H<sub>3</sub>CC=OCOO<sup>-</sup></b>	-597,4	-850	-350,78	$G_{\text{H}_2\text{O}_{\text{Biochem}}} = 85,64 \text{ kJ/mol}; G_{\text{H}^-} = -3,068 - 534,2 - 22,44 + (668,8 + 85,64) = 194,7 \text{ kJ/mol}$
<b>H<sub>3</sub>CC=OCOO<sup>-</sup></b>	-603,7	-433,54	-474,44	
<b>H<sub>3</sub>CC=OCOO<sup>-</sup></b>	<b>-597,04</b>	<b>-846,66</b>	<b>-344,62</b>	$G_{\text{H}_3\text{CHC}(\text{OH})\text{COO}^-} = 534,2 \text{ kJ/mol}; pK_a = 2,5;$
<b>H<sub>3</sub>O<sup>+</sup></b>	-285,81	-3,854	-213,275	
<b>H<sub>2</sub>O</b>	-285,85	69,9565	-237,191	
<b>H<sub>2</sub>O</b>	<b>-286,65</b>	<b>-453,188</b>	<b>-151,549</b>	
<b>H<sub>3</sub>CHC(OH)COO<sup>-</sup></b>	<b>-688,29</b>	<b>-1290,9</b>	<b>-303,4</b>	$G_{\text{H}_3\text{CHC}(\text{OH})\text{COO}^-} = 668,8 \text{ kJ/mol}; pK_a = 3,86;$

$$pK_a = 3,86; \Delta H_c^\circ = 1361,9 \text{ kJ/mol}; G_{\text{H}_3\text{CHC}(\text{OH})\text{COOH}} = 2271 \text{ kJ/mol}; \text{H}_3\text{CHC}(\text{OH})\text{COOH} + 3\text{O}_2\text{gas} = 3\text{CO}_2\text{gas} + 3\text{H}_2\text{O};$$

$$\Delta H_c^\circ = 3G_{\text{CO}_2\text{gas}} + 3G_{\text{H}_2\text{O}} - (G_{\text{H}_3\text{CHC}(\text{OH})\text{COOH}} + 3G_{\text{O}_2\text{gas}}) = 3 \cdot 0 + 3 \cdot 0 - (G_{\text{H}_3\text{CHC}(\text{OH})\text{COOH}} + 3 \cdot 303) = 1361,9 \text{ kJ/mol};$$

$$G_{\text{H}_3\text{CHC}(\text{OH})\text{COOH}} = 3G_{\text{CO}_2\text{gas}} + 3G_{\text{H}_2\text{O}} - (3G_{\text{O}_2\text{gas}}) = 3 \cdot 0 + 3 \cdot 0 - (3 \cdot 303) - 1361,9 = G_{\text{H}_3\text{CHC}(\text{OH})\text{COOH}} = 2271 \text{ kJ/mol};$$

$$\text{Lactic acid Formation 71<sup>st</sup> page } 3\text{C} + 3\text{H}_2\text{gas} + 1,5\text{O}_2\text{gas} \Rightarrow \text{H}_3\text{CHC}(\text{OH})\text{COOH}; G_{\text{H}_3\text{CHC}(\text{OH})\text{COOH}} = -303,4 \text{ kJ/mol [8];}$$

$$\Delta G_{\text{H}_3\text{CHC}(\text{OH})\text{COOH}} = G_{\text{H}_3\text{CHC}(\text{OH})\text{COOH}} - (3G_{\text{Cgraph}} + 3 \cdot G_{\text{H}_2\text{gas}} + 1,5 \cdot G_{\text{O}_2\text{gas}}) = -303,4 \text{ kJ/mol};$$

$$G_{\text{H}_3\text{CHC}(\text{OH})\text{COOH}} = -303,4 + (3 \cdot 91,26 + 3 \cdot 85,6 + 1,5 \cdot 303) = 681,7 \text{ kJ/mol};$$

$$\text{Lactic acid } \text{H}_3\text{CHC}(\text{OH})\text{COOH} + \text{H}_2\text{O} \Leftrightarrow \text{H}_3\text{CHC}(\text{OH})\text{COO}^- + \text{H}_3\text{O}^+; pK_a = 3,86;$$

$$K_{\text{eq}} = [\text{H}_3\text{CHC}(\text{OH})\text{COO}^-] \cdot [\text{H}_3\text{O}^+] / [\text{H}_3\text{CHC}(\text{OH})\text{COOH}] \cdot [\text{H}_2\text{O}] = K_a / [\text{H}_2\text{O}] = 10^{-(3,86)} / 55,3 = 2,5 \cdot 10^{-(6)} = 10^{-(5,603)};$$

$$\Delta G_{\text{eqH}_3\text{CHC}(\text{OH})\text{COOH}} = -R \cdot T \cdot \ln(K_{\text{aq}}) = -8,3144 \cdot 298,15 \cdot \ln(10^{-(5,603)}) / 1000 = 31,98 \text{ kJ/mol}.$$

$$\Delta G_{\text{H}_3\text{CHC}(\text{OH})\text{COO}^-} = G_{\text{H}_3\text{CHC}(\text{OH})\text{COO}^-} + 2G_{\text{H}_3\text{O}^+} - (G_{\text{LacticAc}} + 2G_{\text{H}_2\text{O}}) = G_{\text{Succinat}} + 2 \cdot 22,44 - (681,7 + 2 \cdot 0) = 31,98 \text{ kJ/mol};$$

$$G_{\text{H}_3\text{CHC}(\text{OH})\text{COO}^-} = \Delta G_{\text{H}_3\text{CHC}(\text{OH})\text{COO}^-} - 2G_{\text{H}_3\text{O}^+} + (G_{\text{LacticAc}} + 2G_{\text{H}_2\text{O}}) = 31,98 - 2 \cdot 22,44 + (681,7 + 2 \cdot 0) = 668,8 \text{ kJ/mol};$$

$$\text{Pyruvic acid Formation 71<sup>st</sup> page } 3\text{C} + 2\text{H}_2\text{gas} + 1,5\text{O}_2\text{gas} \Rightarrow \text{H}_3\text{CC}=\text{OCOOH}; \Delta G_{\text{Succinat}} = -344,62 \text{ kJ/mol Alberty};$$

$$\Delta G_{\text{Fumarat}} = G_{\text{Fumarat}} - (3G_{\text{Cgraph}} + 2G_{\text{H}_2\text{gas}} + 1,5 \cdot G_{\text{O}_2\text{gas}}) = -344,62 \text{ kJ/mol};$$

$$G_{\text{Fumarat}} = -344,62 + (3 \cdot 91,26 + 2 \cdot 85,6 + 1,5 \cdot 303) = 554,86 \text{ kJ/mol}; ;$$

$$\text{Pyruvic acid } \text{H}_3\text{CC}=\text{OCOOH} + \text{H}_2\text{O} \Leftrightarrow \text{H}_3\text{CHC}(\text{OH})\text{COO}^- + \text{H}_3\text{O}^+; pK_a = 2,5;$$

$$K_{\text{eq}} = [\text{H}_3\text{CHC}(\text{OH})\text{COO}^-] \cdot [\text{H}_3\text{O}^+] / [\text{H}_3\text{CC}=\text{OCOOH}] \cdot [\text{H}_2\text{O}] = K_a / [\text{H}_2\text{O}] = 10^{-(2,5)} / 55,3 = 2,5 \cdot 10^{-(6)} = 10^{-(4,243)};$$

$$\Delta G_{\text{eqH}_3\text{CC}=\text{OCOOH}} = -R \cdot T \cdot \ln(K_{\text{aq}}) = -8,3144 \cdot 298,15 \cdot \ln(10^{-(4,243)}) / 1000 = 24,22 \text{ kJ/mol}.$$

$$\Delta G_{\text{H}_3\text{CHC}(\text{OH})\text{COO}^-} = G_{\text{H}_3\text{CHC}(\text{OH})\text{COO}^-} + 2G_{\text{H}_3\text{O}^+} - (G_{\text{LacticAc}} + 2G_{\text{H}_2\text{O}}) = G_{\text{Succinat}} + 2 \cdot 22,44 - (554,86 + 2 \cdot 0) = 24,22 \text{ kJ/mol};$$

$$G_{\text{H}_3\text{CHC}(\text{OH})\text{COO}^-} = \Delta G_{\text{H}_3\text{CHC}(\text{OH})\text{COO}^-} - 2G_{\text{H}_3\text{O}^+} + (G_{\text{LacticAc}} + 2G_{\text{H}_2\text{O}}) = 24,22 - 2 \cdot 22,44 + (554,86 + 2 \cdot 0) = 534,2 \text{ kJ/mol};$$

$$\text{NADH} = \text{NAD}^+ + \text{H}^-(\text{H}^+ + 2\text{e}^-); E^\circ_{\text{NADH}} = -0,4095 \text{ V}; \text{absolute Lehninger}; [6]$$

$$\text{Red lactate} + \text{H}_2\text{O} \Leftrightarrow \text{pyruvate} + \text{H}_3\text{O}^+ + \text{H}^-(\text{H}^+ + 2\text{e}^-); \text{absolute potential } E^\circ_{\text{H}_3\text{CHC}(\text{OH})\text{COO}^-} = -0,0159 \text{ V};$$

$$\text{Ox } \text{NAD}^+ + \text{H}^-(2\text{e}^-) = \text{NADH}; E^\circ = -0,4095 \text{ V}; \text{OksRed } \text{NAD}^+ + \text{lactate} + \text{H}_2\text{O} = \text{NADH} + \text{pyruvate} + \text{H}_3\text{O}^+;$$

$$\text{Balanced } n=2=m \text{ with } 2\text{e}^- \text{ electrons } \Delta E^\circ \text{ NAD}^+ \text{ accept electrons from lactate:}$$

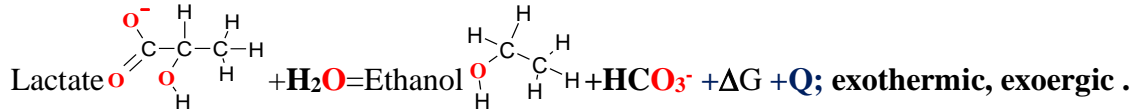
$$\Delta G_{\text{eqAerobic}} = \Delta E^\circ \cdot F \cdot n = (E^\circ_{\text{Red}} - E^\circ_{\text{Ox}}) \cdot F \cdot n = (-0,0159 - (-0,4095)) \cdot 96485 \cdot 2 = (0,3936) \cdot 2 = 75,95 \text{ kJ/mol}$$

$$K_{\text{eqAerobic}} = \text{EXP}(-\Delta G_{\text{eqAerobic}} / R/T) = \text{EXP}(-75950 / 8,3144 / 298,15) = 10^{-13,3};$$

$$K_{\text{eqAerobic}} = \frac{[\text{NADH}] \cdot [\text{pyruvate}^-] \cdot [\text{H}_3\text{O}^+]}{[\text{NAD}^+] \cdot [\text{lactate}^-] \cdot [\text{H}_2\text{O}]} = e^{-\frac{\Delta G_{\text{eqAerobic}}}{R \cdot T}} = e^{-\frac{75950}{8,314 \cdot 298,15}} = 10^{-13,3};$$

$$\Delta G_{\text{Hess}} = \Delta H_{\text{Hess}} - T \cdot \Delta S_{\text{Hess}} = 45,764 - 298,15 \cdot (-0,5479605) = 209,14 \dots \text{ kJ/mol endoergic; formation 62<sup>nd</sup>, 75<sup>th</sup> pages}$$

Pyruvate  $\text{H}_3\text{CC}=\text{OCOO}^-$  decarboxylation  $\text{H}_3\text{CCHO}+\text{HC}\text{O}_3^-$ ;  $\text{H}_3\text{CC}=\text{OCOO}^-+\text{H}_2\text{O}\Delta\text{G}+\text{Q}\Rightarrow\text{H}_3\text{CCHO}+\text{HC}\text{O}_3^-$



$$\Delta\text{G}_{\text{Hess}}=\Delta\text{G}^\circ_{\text{H}_3\text{CCH}_2\text{OH}}+\Delta\text{G}^\circ_{\text{HC}\text{O}_3^-}-\Delta\text{G}^\circ_{\text{H}_2\text{O}}-\Delta\text{G}^\circ_{\text{H}_3\text{CCH}_2\text{OHC}\text{O}_2^-}=\underline{75,2864-544,9688-(-151,549-303,4256)}=-14,71 \text{ kJ/mol}$$

$$\Delta\text{G}_{\text{Alberty}}=\Delta\text{G}_{\text{H}_3\text{CCH}_2\text{OH}}+\Delta\text{G}_{\text{HC}\text{O}_3^-}-\Delta\text{G}_{\text{H}_2\text{O}}-\Delta\text{G}_{\text{H}_3\text{CCH}_2\text{OHC}\text{O}_2^-}=\underline{666,1+46,08-(0+668,8)}=43,38 \text{ kJ/mol}$$

$$\Delta\text{G}_{\text{Alberty\_Biochem}}=\Delta\text{G}_{\text{H}_3\text{CCH}_2\text{OH}}+\Delta\text{G}_{\text{HC}\text{O}_3^-}-\text{G}_{\text{H}_2\text{O\_Biochem}}-\Delta\text{G}_{\text{H}_3\text{CCH}_2\text{OHC}\text{O}_2^-}=\underline{666,1+46,08-(85,64+668,8)}=-42,26 \text{ kJ/mol}$$

$$\Delta\text{H}_{\text{Hess}}=\Delta\text{H}^\circ_{\text{H}_3\text{CCH}_2\text{OH}}+\Delta\text{H}^\circ_{\text{HC}\text{O}_3^-}-\Delta\text{H}^\circ_{\text{H}_2\text{O}}-\Delta\text{H}^\circ_{\text{H}_3\text{CCH}_2\text{OHC}\text{O}_2^-}=-290,77-692,4948-(-286,65-688,29)=-8,325 \text{ kJ/mol}$$

$$\Delta\text{S}_{\text{izkliedes}}=-\Delta\text{H}_{\text{Hess}}/T=8,325/298,15=27,9 \text{ J/K/mol};$$

$$\Delta\text{S}_{\text{Hess}}=\Delta\text{S}^\circ_{\text{H}_3\text{CCH}_2\text{OH}}+\Delta\text{S}^\circ_{\text{HC}\text{O}_3^-}-\Delta\text{S}^\circ_{\text{H}_2\text{O}}-\Delta\text{S}^\circ_{\text{H}_3\text{CCH}_2\text{OHC}\text{O}_2^-}=21,51 \text{ J/mol/K};$$

$$=-1227,764-494,768-(-453,188-1290,852)=21,51 \text{ J/mol/K}....$$

$$\Delta\text{S}_{\text{kopējs}}=\Delta\text{S}_{\text{Hess}}+\Delta\text{S}_{\text{izkliedes}}=21,51+27,9=49,41 \text{ J/mol/K};$$

$$\Delta\text{G}_{\text{Hess}}=\Delta\text{H}_{\text{Hess}}-T\Delta\text{S}_{\text{Hess}}=-8,325-298,15\cdot 0,02151=-14,738 \text{ kJ/mol exoergic}.....$$

$$T\Delta\text{S}_{\text{kopējs}}=0,04941\cdot 298,15 \text{ K}=14,73 \text{ kJ/mol}; \text{ bound } T\Delta\text{S}_{\text{Sn}}; \text{ izkliedes-lost energy patvaļīga}$$

**Lactic acid Formation** 71<sup>st</sup> page  $3\text{C}+3\text{H}_2\text{gas}+1,5\text{O}_2\text{gas}\Rightarrow\text{H}_3\text{CHC}(\text{OH})\text{COOH}$ ;  $\text{G}_{\text{H}_3\text{CHC}(\text{OH})\text{COOH}}=-303,4 \text{ kJ/mol}$  [8];

$$\Delta\text{G}_{\text{H}_3\text{CHC}(\text{OH})\text{COOH}}=\text{G}_{\text{H}_3\text{CHC}(\text{OH})\text{COOH}}-(3\text{G}_{\text{Cgraph}}+3\cdot\text{G}_{\text{H}_2\text{gas}}+1,5\cdot\text{G}_{\text{O}_2\text{gas}})=-303,4 \text{ kJ/mol};$$

$$\text{G}_{\text{H}_3\text{CHC}(\text{OH})\text{COOH}}=-303,4+(3\cdot 91,26+3\cdot 85,6+1,5\cdot 303)=681,7 \text{ kJ/mol};$$

Lactic acid  $\text{H}_3\text{CHC}(\text{OH})\text{COOH}+\text{H}_2\text{O}\rightleftharpoons\text{H}_3\text{CHC}(\text{OH})\text{COO}^-+\text{H}_3\text{O}^+$ ;  $\text{pK}_a=3,86$ ;

$$\text{K}_{\text{eq}}=[\text{H}_3\text{CHC}(\text{OH})\text{COO}^-]\cdot[\text{H}_3\text{O}^+]/[\text{H}_3\text{CHC}(\text{OH})\text{COOH}][\text{H}_2\text{O}]=\text{K}_a/[\text{H}_2\text{O}]=10^{(-3,86)}/55,3=2,5\cdot 10^{(-6)}=10^{(-5,603)};$$

$$\Delta\text{G}_{\text{eqH}_3\text{CHC}(\text{OH})\text{COOH}}=-R\cdot T\cdot \ln(\text{K}_{\text{aeq}})=-8,3144\cdot 298,15\cdot \ln(10^{(-5,603)})/1000=31,98 \text{ kJ/mol} .$$

$$\Delta\text{G}_{\text{H}_3\text{CHC}(\text{OH})\text{COO}^-}=\text{G}_{\text{H}_3\text{CHC}(\text{OH})\text{COO}^-}+2\text{G}_{\text{H}_3\text{O}^+}-(\text{G}_{\text{LacticAc}}+2\text{G}_{\text{H}_2\text{O}})=\text{G}_{\text{Succinat}}+2\cdot 22,44-(681,7+2\cdot 0)=31,98 \text{ kJ/mol};$$

$$\text{G}_{\text{H}_3\text{CHC}(\text{OH})\text{COO}^-}=\Delta\text{G}_{\text{H}_3\text{CHC}(\text{OH})\text{COO}^-}-2\text{G}_{\text{H}_3\text{O}^+}+(\text{G}_{\text{LacticAc}}+2\text{G}_{\text{H}_2\text{O}})=31,98-2\cdot 22,44+(681,7+2\cdot 0)=668,8 \text{ kJ/mol};$$

**CH<sub>3</sub>CH<sub>2</sub>OH** ethanol formation from elements:

$$2\text{C}+3\text{H}_2\text{gas}+1/2\text{O}_2\text{gas}\Rightarrow\text{CH}_3\text{CH}_2\text{OH}; \Delta\text{G}^\circ_{\text{Alberty}}=75,2864 \text{ kJ/mol}; \Delta\text{G}^\circ_{\text{HessCRC}}=-181 \text{ kJ/mol};$$

$$\Delta\text{G}^\circ_{\text{Alberty}}=\text{G}_{\text{CH}_3\text{CH}_2\text{OH}}-(2\text{G}_{\text{Cgraph}}+3\cdot\text{G}_{\text{H}_2\text{gas}}+1/2\cdot\text{G}_{\text{O}_2\text{gas}})=75,2864 \text{ kJ/mol};$$

$$\Delta\text{G}^\circ_{\text{CRC}}=\text{G}_{\text{CH}_3\text{CH}_2\text{OH}}-(2\text{G}_{\text{Cgraph}}+3\cdot\text{G}_{\text{H}_2\text{gas}}+1/2\cdot\text{G}_{\text{O}_2\text{gas}})=-181 \text{ kJ/mol};$$

$$\Delta\text{G}^\circ_{\text{Alberty}}+(2\text{G}_{\text{Cgraph}}+3\cdot\text{G}_{\text{H}_2\text{gas}}+1/2\cdot\text{G}_{\text{O}_2\text{gas}})=75,2864+(2\cdot 91,26+3\cdot 85,6+1/2\cdot 303)=\text{G}_{\text{CH}_3\text{CH}_2\text{OH}}=666,106 \text{ kJ/mol};$$

$$\Delta\text{G}^\circ_{\text{CRC}}+(2\text{G}_{\text{Cgraph}}+3\cdot\text{G}_{\text{H}_2\text{gas}}+1/2\cdot\text{G}_{\text{O}_2\text{gas}})=-181+(2\cdot 91,26+3\cdot 85,6+1/2\cdot 303)=\text{G}_{\text{CH}_3\text{CH}_2\text{OH}}=409,82 \text{ kJ/mol};$$

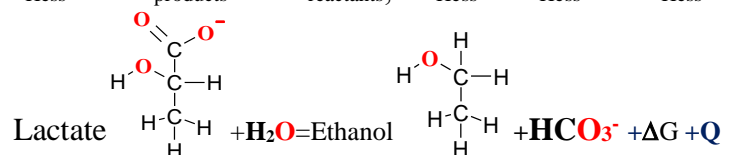
Substance	$\Delta\text{H}^\circ_{\text{H}}$ kJ/mol	$\Delta\text{S}^\circ_{\text{H}}$ J/mol/K	$\Delta\text{G}^\circ_{\text{H}}$ kJ/mol
$\text{H}_3\text{CCH}(\text{OH})\text{COO}^-$	-688,29	-1290,852	-303,4256
$\text{H}_3\text{CCH}(\text{OH})\text{COO}^-$	-686,2	-557,71	-313,70
$\text{H}_3\text{CCH}_2\text{OH}_{\text{aq}}$	-290,77	-1227,764	75,2864
$\text{H}_3\text{CCH}_2\text{OH}_l$	-277,6	160,7	62,96
$\text{H}_2\text{O}$	-285,85	69,9565	-237,191
$\text{H}_2\text{O}$	-286,65	-453,188	-151,549
$\text{HC}\text{O}_3^-$	-689,93	98,324	-586,94
$\text{HC}\text{O}_3^-$	-692,4948	-494,768	-544,9688

**BioThermodynamics06**;  $\text{G}_{\text{H}_2\text{O\_Biochem}}=85,64 \text{ kJ/mol}$ ;

$$(\text{G}_{\text{H}_3\text{O}^+}+\text{G}_{\text{HC}\text{O}_3^-})=22,44+46,08 \text{ kJ/mol};$$

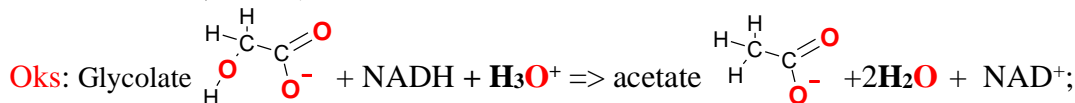
CRC 2010;

$$\Delta\text{S}_{\text{Hess}}=\sum\Delta\text{S}^\circ_{\text{products}}-\sum\Delta\text{S}^\circ_{\text{reactants}};\Delta\text{G}_{\text{Hess}}=\Delta\text{H}_{\text{Hess}}-T\Delta\text{S}_{\text{Hess}}$$



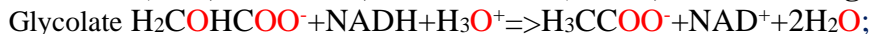
exothermic.....

Oks:  $\text{H}_2\text{COHCOO}^- + \text{H}^+(\text{H}^+ + 2\text{e}^-) + \text{H}_3\text{O}^+ \Rightarrow \text{H}_3\text{CCOO}^- + 2\text{H}_2\text{O}$ ;  $E^\circ_{\text{OxH}_2\text{COHCOO}} = -0,033$  V absolute; [23]



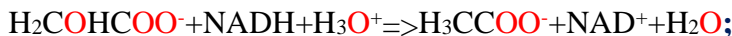
$$\Delta G_{\text{Hess}} = \Delta G^\circ_{\text{CH}_3\text{COO}} + \Delta G^\circ_{\text{NAD}^+} + 2\Delta G^\circ_{\text{H}_2\text{O}} - \Delta G^\circ_{\text{H}_2\text{COHCOO}} - \Delta G^\circ_{\text{NADH}} - \Delta G^\circ_{\text{H}_3\text{O}^+} = -161,8 \text{ kJ/mol};$$

$$= -240,963 + 1112,534 - 2 \cdot 237,191 - (-403,2968 + 1175,5732 - 213,2746) = -161,8 \text{ kJ/mol exoergic} \dots \dots$$



$$\Delta G_{\text{eq}} = (E^\circ_{\text{Red}} - E^\circ_{\text{OxH}_2\text{COHCOO}}) \cdot F \cdot n = (-0,4095 - (-0,033)) \cdot 96485 \cdot 2 = (-0,38) \cdot 96485 \cdot 2 = -72,65 \text{ kJ/mol};$$

Substance	$\Delta H^\circ_{\text{Hess}}$ kJ/mol	$\Delta S^\circ_{\text{Hess}}$ J/mol/K	$\Delta G^\circ_{\text{Hess}}$ kJ/mol
Glyoxylate			
OHCCOOH	-	-	-
OHCCOO-	-	-	-426,588
H <sub>2</sub> COHCOO-	-	-	-403,2968
H <sub>2</sub> COHCOOH	- 651	318,6	-
NADH(aq)	-1036,66	-140,5	-
NADH(aq)	-1041,41	-4081,784	1175,5732
H <sub>3</sub> O <sup>+</sup> (aq)	-285,81	-3,854	-213,2746
NAD <sup>+</sup> (aq)	-1007,48	-183	-
NAD <sup>+</sup> (aq)	-1010,3	-3766,008	1112,534
H <sub>3</sub> CCOOH	-484,09	159,83	-531,743
H <sub>3</sub> CCOO-	-486,84	82,23	-247,83
H <sub>3</sub> CCOO-	-486	85,3	-240,963
H <sub>2</sub> O	-285,85	69,9565	-237,191
H <sub>2</sub> O	,65	-453,188	-151,549



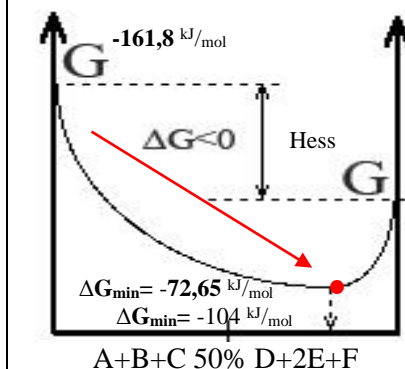
$$G_{\text{OHCCOOH}} = -426,588 + (2 \cdot 91,26 + 85,6 + 1,5 \cdot 303) = 296,032 \text{ kJ/mol}$$

$$G_{\text{OHCCOO}} = \Delta G_{\text{eqOHCCOOH}} - G_{\text{H}_3\text{O}^+} + (G_{\text{OHCCOOH}} + G_{\text{H}_2\text{O}}) = 305,6 \text{ kJ/mol}$$

$$G_{\text{OHCCOO}} = \Delta G_{\text{eqOHCCOOH}} - G_{\text{H}_3\text{O}^+} + (G_{\text{OHCCOOH}} + G_{\text{H}_2\text{O}}) = 414,3 \text{ kJ/mol}$$

$$G_{\text{H}_2\text{COHCOOH}} = -403,2968 + (2 \cdot 91,26 + 2 \cdot 85,6 + 1,5 \cdot 303) = 404,9232 \text{ kJ/mol}$$

Exothermic, exoergic reduction Hess free energy change -161,8 negative, but minimized reaching  $\Delta G_{\text{min}} = \Delta G_{\text{eq}} = -72,65$  or -104 kJ/mol equilibrium mixture. Le Chatelier principle is Prigogine attractor free energy change minimum  $\Delta G_{\text{min}}$  reaching.



Glyoxylic acid Formation 61<sup>st</sup> page  $2\text{C} + \text{H}_2\text{gas} + 1,5\text{O}_2\text{gas} \Rightarrow \text{OHCCOOH}$ ;  $\Delta G_{\text{OHCCOOH}} = -426,588$  kJ/mol [8];

$$\Delta G_{\text{OHCCOOH}} = G_{\text{OHCCOOH}} - (2G_{\text{Cgraph}} + G_{\text{H}_2\text{gas}} + 1,5 \cdot G_{\text{O}_2\text{gas}}) = -426,588 \text{ kJ/mol};$$

$$G_{\text{OHCCOOH}} = -426,588 + (2 \cdot 91,26 + 85,6 + 1,5 \cdot 303) = 296,032 \text{ kJ/mol};$$

Glyoxylic acid  $\text{OHCCOOH} + \text{H}_2\text{O} \rightleftharpoons \text{OHCCOO}^- + \text{H}_3\text{O}^+$ ;  $pK_{a1} = 3,32$ ; Wikipedia

$$K_{\text{eq}} = \frac{[\text{OHCCOO}^-][\text{H}_3\text{O}^+]}{[\text{OHCCOOH}][\text{H}_2\text{O}]} = K_a / [\text{H}_2\text{O}] = 10^{-(3,32)} / 55,3 = 8,655 \cdot 10^{-(6)} = 10^{-(5,063)};$$

$$\Delta G_{\text{eqOHCCOOH}} = -R \cdot T \cdot \ln(K_{\text{aq}}) = -8,3144 \cdot 298,15 \cdot \ln(10^{-(5,063)}) / 1000 = 31,98 \text{ kJ/mol}.$$

$$\Delta G_{\text{eqOHCCOOH}} = G_{\text{OHCCOO}} + G_{\text{H}_3\text{O}^+} - (G_{\text{OHCCOOH}} + G_{\text{H}_2\text{O}}) = G_{\text{OHCCOO}} + 22,44 - (296,032 + 0) = 31,98 \text{ kJ/mol};$$

$$G_{\text{OHCCOO}} = \Delta G_{\text{eqOHCCOOH}} - G_{\text{H}_3\text{O}^+} + (G_{\text{OHCCOOH}} + G_{\text{H}_2\text{O}}) = 31,98 - 22,44 + (296,032 + 0) = 305,6 \text{ kJ/mol};$$

Glycolic acid Formation 61<sup>st</sup> page  $2\text{C} + 2 \cdot \text{H}_2\text{gas} + 1,5\text{O}_2\text{gas} \Rightarrow \text{H}_2\text{COHCOOH}$ ;  $\Delta G_{\text{H}_2\text{COHCOOH}} = -403,2968$  kJ/mol [8];

$$\Delta G_{\text{H}_2\text{COHCOOH}} = G_{\text{H}_2\text{COHCOOH}} - (2G_{\text{Cgraph}} + 2G_{\text{H}_2\text{gas}} + 1,5 \cdot G_{\text{O}_2\text{gas}}) = -403,2968 \text{ kJ/mol};$$

$$G_{\text{H}_2\text{COHCOOH}} = -403,2968 + (2 \cdot 91,26 + 2 \cdot 85,6 + 1,5 \cdot 303) = 404,9232 \text{ kJ/mol};$$

Glycolic acid  $\text{H}_2\text{COHCOOH} + \text{H}_2\text{O} \rightleftharpoons \text{H}_2\text{COHCOO}^- + \text{H}_3\text{O}^+$ ;  $pK_{a1} = 3,83$ ; Wikipedia

$$K_{\text{eq}} = \frac{[\text{H}_2\text{COHCOO}^-][\text{H}_3\text{O}^+]}{[\text{H}_2\text{COHCOOH}][\text{H}_2\text{O}]} = K_a / [\text{H}_2\text{O}] = 10^{-(3,83)} / 55,3 = 2,675 \cdot 10^{-(6)} = 10^{-(5,573)};$$

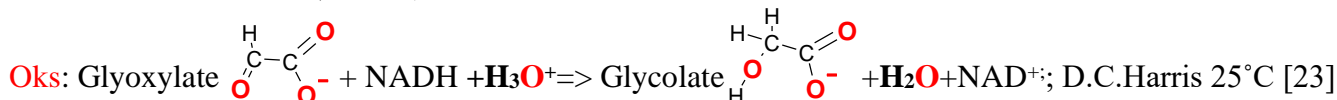
$$\Delta G_{\text{eqOHCCOOH}} = -R \cdot T \cdot \ln(K_{\text{aq}}) = -8,3144 \cdot 298,15 \cdot \ln(10^{-(5,573)}) / 1000 = 31,81 \text{ kJ/mol}.$$

$$\Delta G_{\text{eqOHCCOOH}} = G_{\text{OHCCOO}} + G_{\text{H}_3\text{O}^+} - (G_{\text{OHCCOOH}} + G_{\text{H}_2\text{O}}) = G_{\text{OHCCOO}} + 22,44 - (404,9232 + 0) = 31,81 \text{ kJ/mol};$$

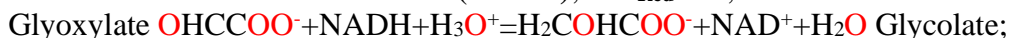
$$G_{\text{OHCCOO}} = \Delta G_{\text{eqOHCCOOH}} - G_{\text{H}_3\text{O}^+} + (G_{\text{OHCCOOH}} + G_{\text{H}_2\text{O}}) = 31,81 - 22,44 + (404,9232 + 0) = 414,3 \text{ kJ/mol};$$

Nernst's half reaction glycolate +  $\text{H}_2\text{O} =$  Glyoxylate +  $\text{H}^+(\text{H}^+ + 2\text{e}^-) + \text{H}_3\text{O}^+$ ; D.C.Harris 25°C [23]

Oks:  $\text{OHCCOO}^- + \text{H}^+(\text{H}^+ + 2\text{e}^-) + \text{H}_3\text{O}^+ \Rightarrow \text{H}_2\text{COHCOO}^- + \text{H}_2\text{O}$ ;  $E^\circ_{\text{H}_2\text{COHCOO}} = 0,1305$  V absolute; [23]



Nernst's half reaction Red:  $\text{NADH} = \text{NAD}^+ + \text{H}^+(\text{H}^+ + 2\text{e}^-)$ ;  $E^\circ_{\text{Red}} = -0,4095$  V David Harris absolute [22]



$$\Delta G_{\text{Hess}} = \Delta G^\circ_{\text{H}_2\text{COHCOOH}} + \Delta G^\circ_{\text{NAD}^+} + \Delta G^\circ_{\text{H}_2\text{O}} - \Delta G^\circ_{\text{H}_2\text{COHCOO}} - \Delta G^\circ_{\text{NADH}} - \Delta G^\circ_{\text{H}_3\text{O}^+} = -63,66 \text{ kJ/mol};$$

$$= -403,2968 + 1112,534 - 237,191 - (-426,588 + 1175,5732 - 213,2746) = -63,66 \text{ kJ/mol exoergic} \dots \dots \dots;$$

$$\Delta G_{\text{min}} = \Delta G_{\text{eq}} = (E^\circ_{\text{eqNernst\_NADH}} - E^\circ_{\text{H}_2\text{COHCOO}}) \cdot F \cdot n = (-0,4095 - 0,1305) \cdot 96485 \cdot 2 = (-0,54) \cdot 96485 \cdot 2 = -104,2 \text{ kJ/mol};$$



**Nernst's potential  $O_{2\text{aqua}}/H_2O$  red-ox system biochemical mechanism of acidosis and oxidative stress**  
(forced oxidizing agent power by potential E increase)

Note: Oxidative stress causes **non enzymatic** oxidation in multiple radical chain and reactions of parallel product formations to contaminate and destroy the organism! Destructive hazard for life!

Water medium (blood plasma) oxygen is strong oxidant absolute potential  $E^\circ_{O_2} = 1,0868$  V oxidized form free electrons reduced form by half reaction:  $O_{2\text{aqua}} + 4H_3O^+ + 4e^- \rightleftharpoons 6H_2O$ ;

Free energy content is gas and water solubility product  $G_{O_{2\text{aqua}}} = G_{O_{2\text{gas}}} + G_{O_{2\text{sk}}} = 303.1 + 26.58 = 330$  kJ/mol ;  
 $G_{H_3O^+ + OH^-} = G_{H_3O^+} + G_{OH^-} = 22.44 + 77.36 = 99.8$  kJ/mol of  $H_2O + H_2O \rightleftharpoons H_3O^+ + OH^-$

Biochemistry oxygen  $O_{2\text{aqua}}$  decreases free energy content  $G_{O_{2\text{aqua}}} = 329.7$  kJ/mol to  $G_{O_{2\text{Biochemistry}}} = 78.08$  kJ/mol.  
Concentration arterial  $[O_{2\text{aqua}}] = 6 \cdot 10^{-5}$  M and pH=7.36 concentration  $[H_3O^+] = 10^{-7.36}$  M decrease potential:

$$E_{O_2} = E^\circ + 0.0591/4 \cdot \log([O_{2\text{aqua}}] \cdot [H_3O^+]^4 / [H_2O]^6) = 1.0868 + 0.0591/4 \cdot \log(6 \cdot 10^{-5} \cdot 10^{-29.44} / 55.346^6) = 0.4346$$
 V with

difference  $\Delta E_{\text{arterial}} = E^\circ - E_0 = 1.0865 - 0.4346 = -0.652$  V;  $\Delta G_{\text{arterial}} = \Delta E_{H_2O} \cdot F \cdot n = -0.652 \cdot 96485 \cdot 4 / 1000 = -251.6$  kJ/mol.  
Solubility product value  $O_{2\text{gas AIR}} + H_2O \xrightarrow{\text{Aquaporins}} O_{2\text{Blood}}$  increases about  $G_{O_{2\text{sk}}} = 26.58$  kJ/mol:

$$\frac{[O_{2\text{aqua}}]}{[O_{2\text{gas}}] \cdot [H_2O]} = K_{\text{sk}} = 2.205 \cdot 10^{-5}. G_{O_{2\text{sk}}} = -R \cdot T \cdot \ln(K_{\text{sk}}) = -8.3144 \cdot 298.15 \cdot \ln(2.205 \cdot 10^{-5}) = 26.58$$
 kJ/mol.

Free energy protolysis decreases  $G_{O_{2\text{Biochem\_arterial}}} = G_{O_{2\text{aqua}}} + G_{O_{2\text{sk}}} + \Delta G_{\text{arterial}} = 303.1 + 26.58 - 251.6 = 78.08$  kJ/mol  
and oxygen becomes fire safe biochemical oxidant, forming arterial concentration  $[O_{2\text{aqua}}] = 6 \cdot 10^{-5}$  M as safe Bioenergetic sustaining normal isooxia. [3];

Oxygen solubility Prigogine attractor free energy change Hess law solution is exothermic and endoergic

$O_{2\text{air}} + H_2O \rightleftharpoons O_{2\text{aqua}}$  ;  $[O_{2\text{air}}] = 0.2095$  oxygen mol fraction in air, in water  $[O_{2\text{aqua}}]/[H_2O]$ :

$\Delta G_H = \Delta G^\circ_{O_{2\text{aqua}}} - \Delta G^\circ_{H_2O} - \Delta G^\circ_{O_{2\text{gas}}} = 16.4 - (0 - 151.549) = 168$  kJ/mol **endoergic**;

$\Delta G_{\text{sk}} = -R \cdot T \cdot \ln(K_{\text{sk}}) = -8.3144 \cdot 298.15 \cdot \ln(2.205 \cdot 10^{-5}) = -8.3144 \cdot 298.15 \cdot 6.414 = 26.58$  kJ/mol

$[O_2]$  solubility Hess free energy change is positive  $\Delta G_{\text{Hess}} = \Delta G_{\text{solubility}} = 168$  kJ/mol ,

but minimized to  $\Delta G_{\text{min}} = \Delta G_{\text{sk}} = 26.58$  kJ/mol reaching solubility product

$$\text{equilibrium mixture } K_{\text{sk}} = \frac{[O_{2\text{aqua}}]}{[O_{2\text{air}}] \cdot [H_2O]} = 2.205 \cdot 10^{-5} = 10^{-4.66}.$$

Equilibrium reaching is Prigogine attractor free energy change minimum  $\Delta G_{\text{min}}$  .

Free energy change minimum  $\Delta G_{\text{min}}$  reaching establishes equilibrium. [53rd page](#).

Zero osmolar  $C_{\text{osm}} = 0$  M and ionic force  $I = 0$  M in distilled water from air 20.95% solubility is:

$$[O_{2\text{water}}] = K_{\text{sk}} \cdot [O_{2\text{air}}] \cdot [H_2O] = 2.205 \cdot 10^{-5} \cdot 0.2095 \cdot 55.3 = 2.5567 \cdot 10^{-4}$$
 M.

ELSEVIER, Rotating Electrode Method and Oxygen reduction Electrocatalysts, 2014, p.1-31,

1. WeiXinga, MinYinb, QingLv, YangHub, ChangpengLiub, JiujunZhangc. Pure 1atm mol fraction  $[O_{2\text{gas}}] = 1$ .

Osmolar  $C_{\text{osm}} = 0.305$  M, ionic force  $I = 0.25$  M, air oxygen 20.95% conditions dissolve  $[O_{2\text{aqua}}] = 9.768 \cdot 10^{-5}$  M.

Therefore physiologic equilibrium constant is  $K_{O_{2\text{blood}}} = [O_{2\text{aqua}}] / [O_{2\text{air}}] = 9.768 \cdot 10^{-5} / 0.2095 = 4.663 \cdot 10^{-4} = 10^{-3.3314}$ .

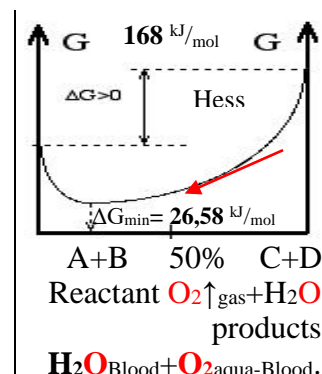
Arterial  $[O_{2\text{aqua}}] = 6 \cdot 10^{-5}$  M versus venous  $[O_{2\text{aqua}}] = 0.426 \cdot 10^{-5}$  M determines  $pK_{O_{2\text{Arterial}}} = 3.3314$ . Oxygen molecules cross through aquaporins membranes against gradient of osmolar concentration.

Ox:  $O_{2\text{aqua}} + 4H_3O^+ + 4e^- \rightleftharpoons 6H_2O$ ;  $E^\circ_{O_2} = 1.0865$  Volts; Red:  $4H(\text{Pt}) + 4H_2O \rightleftharpoons 4H_3O^+ + 4e^-$ ;  $E^\circ_H = -0.2965$  V.

$O_{2\text{aqua}} + 4H(\text{Pt}) = 2H_2O$ ;  $\Delta G_{\text{eq}} = (E^\circ_H - E^\circ_{O_2}) \cdot F \cdot 1 \cdot 4 = (-0.2965 - 1.0868) \cdot 96485 \cdot 4 = -1,383 \cdot 96485 \cdot 4 / 1000 = -533,9$  kJ/mol;

Equilibrium value  $\Delta G_{\text{eq}2H_2O} = 2G_{H_2O} - 4G_{H(\text{Pt})} - G_{O_{2\text{aqua}}} = 2 \cdot 0 - (4 \cdot G_{H(\text{Pt})} + 330) = -533,9 = 2 \cdot 266,9$  kJ/mol expresses metal free energy  $G_{H(\text{Pt})} = (2G_{H_2O} - \Delta G_{\text{eq}2H_2O} - G_{O_{2\text{aqua}}}) / 4 = (2 \cdot 0 + 533,9 - 330) / 4 = 204,2 / 4 = 51,05$  kJ/mol .

$H_{2\text{aq}} + 2H_2O \rightleftharpoons 2H_3O^+ + 2e^- + H_2O$ ; Nernst's half reaction



$\Delta G_{\text{Hess}_H3O^+} = G_{H2aq} + 2G_{H2O} - (2G_{H3O^+} + G_{H2O}) = 103,24 + 2 \cdot 0 - (2 \cdot 22,44 - 2 \cdot 0) = 58,36 \text{ kJ/mol}$ ; and graphite electrode absolute potential  $E^\circ_{H3O^+} = 58360/96485/2 = 0,302 \text{ V}$  oxidizes hydrogen and liberate (Pt) lattice.

**Red:**  $2H(Pt) + 2H_2O \leftrightarrow 2H_3O^+ + 2e^-$ ;  $E^\circ_{H^+} = -0,2965 \text{ V}$ ; **Ox+Red** summary  $2H(Pt) + H_2O \leftrightarrow H_{2aq}$ ;

Ox:  $2H_3O^+ + H_2O + 2e^- \leftrightarrow H_{2aq} + 2H_2O$ ;

Red:  $2H(Pt) + 2H_2O \leftrightarrow 2H_3O^+ + 2e^-$ ;

$2H(Pt) + H_2O \leftrightarrow H_{2aq}$ ;

$\Delta E^\circ_{eqH3O^+H(Pt)} = -0,2965 - 0,302 = -0,5985 \text{ V}$ ;  $\Delta G_{eqH3O^+H(Pt)} = \Delta E^\circ_{eqH3O^+H(Pt)} \cdot F \cdot 2 = -0,5985 \cdot 96485 \cdot 2 = -115,5 \text{ kJ/mol}$ ;

$\Delta G_{eqH3O^+H(Pt)} = G_{H2aq} + G_{H2O} - 2G_{H(Pt)} = 103,24 + 0 - 2 \cdot 51,05 = 1,14 \text{ kJ/mol}$ .

$\Delta G_{eqH3O^+H(Pt)} = G_{H2aq} + G_{H2O\_Biochem} - 2G_{H(Pt)} = 103,24 + 85,6 - 2 \cdot 51,05 = 86,74 \text{ kJ/mol}$ .

Platinum crystal lattice is indifferent referring to zero free energy for  $G_{H2O} = G_{CO2gas} = G_e = 0 \text{ kJ/mol}$ ,

Reduction of sulfur Ox:  $S_{rombisks} + 2H_3O^+ + 2e^- = H_2S_{aq} + 2H_2O$ ;  $E^\circ_s = -0,0515 \text{ V}$ ;

$S_{rombisks} + 2H(Pt) \leftrightarrow H_2S_{aq}$ ;

$\Delta G_{eq} = (E^\circ_H - E^\circ_s) \cdot F \cdot 1 \cdot 2 = (-0,2965 - (-0,0515)) \cdot 96485 \cdot 2 = -0,245 \cdot 96485 \cdot 2/1000 = -47,3 \text{ kJ/mol}$ ;

$G_{H2S_{aq}} = \Delta G_{HessH2S} + (2G_{H(Pt)} + G_{S_{rombisks}}) = -47,3 + (2 \cdot -219 - 85,64) = -571 \text{ kJ/mol}$ . [2nd page](#).

### Abstrakts.

Uz Alberti bāzēts absolūtās brīvās enerģijas saturs  $G_{H2gas} = 85,6 \text{ kJ/mol}$  gāzei,  $G_{H2aqua} = 103 \text{ kJ/mol}$  ūdenim un  $G_{H(Pt)} = 51 \text{ kJ/mol}$  [metālam](#) ūdeņradim pie nulles atskaites  $G_{H2O} = G_{CO2gas} = 0 \text{ kJ/mol}$  fona enerģijas ūdenim un oglekļa dioksīda  $CO_{2gas}$  gāzei. [8,15] Metāla ūdeņraža nulles klasiskā standarta potenciāla atskaite tiek izmantota tā hidroksionija katjona  $[H_3O^+] = 1,01 \text{ M}$  koncentrācija sērskābes  $[H_2SO_4] = 1 \text{ M}$  šķīdumā ar blīvumu  $1,061 \text{ g/mL}$ . Kopš 1920. gada Nernsta Nobela prēmijas ķīmijā saņemšanas visas elektroķīmijas sērijas reducētāju oksidēšanas pusreakciju standarta potenciāli ir noteikti attiecībā pret ūdeņraža metāla pusreakcijas klasisko standarta potenciālu  $E^\circ_H$  nulle. [1,15] Skābekļa, oglekļa dioksīda un ūdens protolīzes funkcionālās aktivitātes kvantitatīvie pētījumi atklāj ģenerētus daudzveidīgus Dzīvības pašorganizējošus atraktorus: ūdens  $[H_2O] = 55,3 \text{ mol/Litrā}$  koncentrāciju,  $pH = 7,36$ , enzīma karbo anhidrāzes (CA) reaktivāte, gaisa skābekļa līmenis  $20,95 \%$ , osmolārā koncentrācija  $0,305 \text{ M}$ , jonu spēks  $0,25 \text{ M}$ , temperatūra  $310,15 \text{ K}$  grādi utt. . [1,15]

Liela ātruma protolīze ūdenī padara skābekli ugunsdrošu, CA funkcionāli aktivizē oglekļa dioksīdu, reaģējot ar divām ūdens molekulām, veidojot  $H_3O^+ + HCO_3^-$  koncentrācijas gradientus abpus membrānei osmozei pretēji koncentrācijas gradientiem bet protonu un bikarbonāta jonu transportēšanai lejup cauri protonu un bikarbonātu jonu kanāliem.

Iepriekšējās publikācijas atklāj neaizstājamu ūdens un hidroksionija uzskaiti līdzsvara reakciju termodinamiskajās izpausmēs, ieskaitot protolīzi un elektroķīmijas Nernsta pusreakcijas. [8,14,15] Pētījumi sasniedz metāla ūdeņraža termodinamiskā standarta potenciāla atsauces vērtību  $0,10166 \text{ Volti}$ . Alberty vārdā sniegtie dati par ūdeņraža brīvo enerģiju  $G_{H2gas} = 85,6 \text{ kJ/mol}$ ,  $G_{H2aqua} = 103 \text{ kJ/mol}$  ir atklājies **absolūtais** standarta **potenciāls**  $E^\circ_H = -0,2965 \text{ Volts}$  kā elektroda termodinamiskā atskaites vērtība ar absolūtās brīvās enerģijas izmaiņas vērtību  $\Delta G_{eq} = -28,6 \text{ kJ/mol}$ .

**Atslēgas vārdi:** Fizikālā ķīmija; Elektroķīmija; Termodinamika; Atraktori; Bioķīmija.

**Nernsta absolūtā potenciāla  $O_{2(aq)} / H_2O$  |  $H(Pt) / H_3O^+$  un  $H_2O_2 / H_2O$  |  $H_2O_2 / O_2$  studijas**

Ox oksidanta reaktanta pus reakcija:  $O_{2(aq)} + 4H_3O^+ + 4e^- \rightleftharpoons 6 H_2O$ ;  $G_{O_{2(aq)}}=330$  kJ/mol;  $E^\circ_{O_2}=0,9851$  V;

Red reaktanta reaktanta pus reakcija:  $4H(Pt)+4H_2O \rightleftharpoons 4 H_3O^++4e^-$ ; metāls ūdeņradis  $G_{H(Pt)}=51,05$  kJ/mol;

$$O_{2(aq)}+4H(Pt) \rightleftharpoons 2H_2O; \Delta G_{eq}=2G_{H_2O}-4G_{H(Pt)}-G_{O_{2(aq)}}=(2*0-4G_{H(Pt)}-330)=-533,886 \text{ kJ/mol}$$

$$E_{O_2}=E^\circ_{O_2}+0.0591/4 \cdot \lg([O_{2(aq)}] \cdot [H_3O^+]^4/[H_2O]^6)=1,0868+0.0591/4 \cdot \lg([O_{2(aq)}] \cdot [H_3O^+]^4/[H_2O]^6);$$

$$E_H=E^\circ_H+0.0591 \cdot \lg([H_3O^+]/[H_2O])=-0.2965 \text{ V} +0.0591 \cdot \lg([H_3O^+]/[H_2O]); E^\circ_H=-0.2965 \text{ V}.$$

$$\text{Gāze } O_{2(g)}+2H_{2(g)} \rightleftharpoons 2H_2O; \Delta G_{Hess2H_2O}=2\Delta G^\circ_{H_2O}-(2\Delta G^\circ_{H_2(g)}+\Delta G^\circ_{O_{2(g)}})=2* -237.19-(2*0+0)=2* -237.19=-546.4 \text{ kJ/mol}$$

$$O_{2(aq)}+2H_{2(aq)} \rightleftharpoons 2H_2O; \Delta G_{Alberty2H_2O}=2G_{H_2O}-2G_{H_{2(aq)}}-G_{O_{2(aq)}}=2*0-(2*103.24+330)=-536,48=2*268,24 \text{ kJ/mol};$$

Ūdeņraža Alberty R.A. Biochemical Thermodynamic's 1-463. (2006). brīvā enerģija  $G_{H_{2(aq)}}=103$  kJ/mol

Viela	$\Delta H^\circ_H, \text{kJ/mol}$	$\Delta S^\circ_H, \text{J/mol/K}$	$\Delta G^\circ_H, \text{kJ/mol}$
$H_2O$	-285.85	69.9565	-237.191
$H_2O$	<b>-286.65</b>	<b>-453.188</b>	<b>-151.549</b>
$H_3O^+$	-285.81	-3.854	-213.2746
$H_2(aq)$	23.4	-130	99.13
$O_{2(aq)}$	<b>-11.70</b>	<b>-94.2</b>	<b>16.4</b>
$O_{2(aq)}$	-11.715	110.876	16.4

$$\Delta G_{Hess}=2\Delta G^\circ_{H_2O}-4\Delta G_{H(Pt)}-\Delta G^\circ_{O_{2(aq)}}=-694,98=2* -347,5 \text{ kJ/mol};$$

$$=2* -237,191-(4*51,05+16,4)=-694,98=2*347,5 \text{ kJ/mol. CRC 2010}$$

$$\Delta G_{eq}=-533,886 \text{ kJ/mol}; \Delta G_{Hess}=-689 \text{ kJ/mol}$$

reaction  $4H(Pt) + O_{2(aq)} \rightleftharpoons 2 H_2O$ ; absolūtā values

$$|\Delta G_{eq}=-494,62 \text{ kJ/mol}| < |\Delta G_{Hess}=-689 \text{ kJ/mol}|;$$

$[H_2O]^6$  logaritms no  $E^\circ_{O_2}$  classic=1,229 V termodinamiskais potenciāls  
 $E^\circ=1,383+0,10166=1.485$  V absolūtais  $E^\circ=1,485-0,3982=1,0868$  V

$$\Delta G_{eqOxRed}=(E^\circ_H-E^\circ_{O_2}) \cdot F \cdot 1 \cdot 4=(-0.2965-1,0868) \cdot 96485 \cdot 4=-1,383 \cdot 96485 \cdot 4/1000=-533,9=2* -266,9 \text{ kJ/mol};$$

$$K_{eq2H_2O}=\exp(-\Delta G_{OxRed}/R/T)=\exp(533870,8/8,3144/298,15)=\exp(215,363)=10^{93,53}$$

$$G_{H(Pt)}=(2G_{H_2O}-\Delta G_{eq2H_2O}-G_{O_{2(aq)}})/4=(2*0+533,871-330)/4=204,2/4=51,05 \text{ kJ/mol}$$

Eksotermiska un eksoergiska  $O_{2(aq)}$  reducēšana ar metālisku ūdeņradi  $4H(Pt)$  un  $H_2O_2$  dismutācijas Hesa brīvās enerģijas izmaiņa negatīva

$$\Delta G_{Hess2H_2O}=-347,5 \dots \text{ kJ/mol}, \Delta G_{Hess_{H_2O_2}}=-242,5 \dots \text{ kJ/mol}, \text{ bet minimizējas}$$

$$\text{sasniedzot līdzsvara } \Delta G_{eq2H_2O}=-247 \text{ kJ/mol and } \Delta G_{eqStandard}=-238,5 \dots \text{ kJ/mol}$$

$$\text{maisījuma konstantes } K_{eq2H_2O}=10^{86,65} \dots \text{ un } K_{eqStandard}=10^{38,35} \dots$$

Minimums  $\Delta G_{min}$  ir Prigožina atraktors. Brīvās enerģijas izmaiņas minimuma sasniegšanā iestājas līdzsvara stāvoklis.

Absolūtā potenciālu skalā Nernsta pus reakciju standarta potenciāli ir:

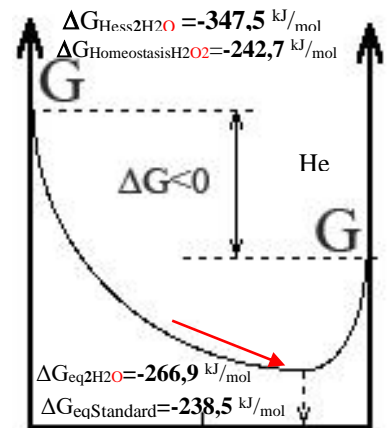
$$\text{Red } H_2O_2+2 H_2O-2 e^-=O_{2(aq)}+2 H_3O^+; E^\circ_{H_2O_2}=0.4495 \text{ V Alberta University};$$

$$\text{Oks } H_2O_2+2 H_3O^++2 e^-=4 H_2O; E^\circ_{Ox}=1,6855 \text{ V Suhotina};$$

$$2H_2O_{2(aq)} \rightleftharpoons O_{2(aq)}+2H_2O+Q+\Delta G;$$

Reaktanti  $4H(Pt)+ O_{2(aq)}$  un produkti  $2H_2O$

Reaktanti  $2H_2O_{2(aq)}$  un produkti  $O_{2(aq)}+2H_2O$



4A+B 50% 2D  
2A 50% B+2C

$$\Delta G_{Hess}=G_{O_{2(aq)}}+2*G_{H_2O}-2*G_{H_2O_2}=16,4+2* -151,549-2* -134=-18,7 \text{ kJ/mol};$$

$$\Delta G_{HessCRC}=G_{O_{2(aq)}}+2*G_{H_2O}-2*G_{H_2O_2}=16,4+2* -237,19-2* -134=-189.98 \text{ kJ/mol};$$

$$\Delta G_{eqStandard}=(E_{Red}-E_{Ox}) \cdot F \cdot n=(0,4495-1,6855) \cdot 96485 \cdot 2=(-1,24) \cdot 96485 \cdot 2=-238,5 \text{ kJ/mol};$$

$$\Delta G_{AlbertyStandard}=G_{O_2Biochem_{arteria}}+2*G_{H_2OBioChemistry}-2*G_{H_2O_2}=78,08+2*85,64-2*284,25=-238,5 \text{ kJ/mol}; \text{ Alberty}$$

$$2G_{H_2O_2}=G_{O_{2(aq)}}+2*G_{H_2O}+\Delta G_{AlbertyStandard}=330+2*0+218,9=2*284,25=548,9 \text{ kJ/mol};$$

$$K_{eqStandard}=\frac{[O_2]_{aq} \cdot [H_2O]^2}{[H_2O_2]_{aq}^2}=K_{H_2O_2}=\exp(-\Delta G_{eq}/R/T)=\exp(238510/8.3144/298.15)=10^{41,75} \dots$$

$$\text{Red: } E_{oH_2O_2}=E^\circ_{H_2O_2}+0.0591/2 \cdot \lg(O_{2(aq)} \cdot [H_3O^+]^2/[H_2O_2]/[H_2O]^2)=0.4495+0.0591/2 \cdot \lg(6 \cdot 10^{-5} \cdot 10^{(-7.36 \cdot 2)}/1/55.3^2)=-0.213 \text{ V}$$

$$\text{Ox: } E_{oOx}=E^\circ_{H_2O_2Ox}+0.0591/2 \cdot \lg([H_2O_2] \cdot [H_3O^+]^2/[H_2O]^4)=1,6855+0.0591/2 \cdot \lg(1 \cdot 10^{(-7.36 \cdot 2)}/55.3^4)=1,0445 \text{ V}$$

$$\text{Homeostāze: } \Delta G_{eqBioChem}=(E_{Red}-E_{Ox}) \cdot F \cdot n=(-0.2132-1,0445) \cdot 96485 \cdot 2=(-1,258) \cdot 96485 \cdot 2=-242,7 \text{ kJ/mol};$$

$$1. \Delta H_{Hess}=\Delta H^\circ_{O_2}+2\Delta H^\circ_{H_2O}-2\Delta H^\circ_{H_2O_2}=-11.7-2*286.65-(2* -191.99)=-201.02 \text{ kJ/mol}=-11.7-2*285.85-(2* -191.17)=-201.06 \text{ kJ/mol}$$

$$2. \Delta S_{izkliedes}=-\Delta H_H/T=(-201.02)/298.15=674.2 \text{ J/mol/K}; \Delta S_{izkliedes}=-\Delta H_H/T=(-201.06)/298.15=674.36 \text{ J/mol/K};$$

$$\Delta S_{Hess}=\Delta S^\circ_{O_2}+2\Delta S^\circ_{H_2O}-2\Delta S^\circ_{H_2O_2}=-94.2+2* -453.188-(2* -481.688)=-37.2 \text{ J/mol/K};$$

$$\Delta S_{Hess}=\Delta S^\circ_{O_2}+2\Delta S^\circ_{H_2O}-2\Delta S^\circ_{H_2O_2}=110.876+2*69.9565-(2*143.9)=-37 \text{ J/mol/K};$$

$$2. \Delta S_{kopējs}=\Delta S_H+\Delta S_{izkliedes}=-37.2+674.2=637 \dots \text{ J/mol/K } \Delta S_{kopējs}=-37.011+674.36=637.35 \dots \text{ J/mol/K};$$

$$4. \Delta G_{Hess}=\Delta H_H-T \cdot \Delta S_H=-201.02-298.15 \cdot -0.0372=-189.9 \text{ kJ/mol exoergic patvaļīga.}$$

$$\Delta G_{Hess}=\Delta H_H-T \cdot \Delta S_H=-201.06-298.15 \cdot -0.037=-190 \text{ kJ/mol};$$

$$T \cdot \Delta S_{kopējs}=0.637 \cdot 298.15=189.9 \text{ kJ/mol}; T \cdot \Delta S_{kopējs}=0.63735 \cdot 298.15=190 \text{ kJ/mol};$$

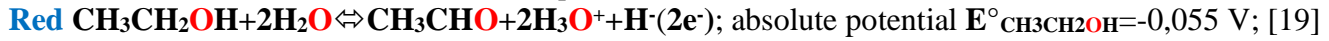
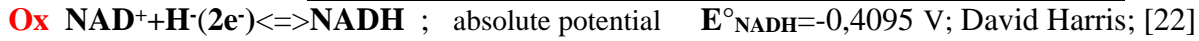
**Nernst's potential** studies reducing with vitamin B<sub>3</sub> ethanal H<sub>3</sub>CCH=O and oxidising H<sub>3</sub>CCH<sub>2</sub>OH ethanol



$\Delta G_{Hess} = \Delta G^{\circ}_{H_3O} + \Delta G^{\circ}_{CH_3CHO} + \Delta G^{\circ}_{NADH} - \Delta G^{\circ}_{CH_3CH_2OH} - \Delta G^{\circ}_{H_2O} - \Delta G^{\circ}_{NAD^+} = 159.1 \text{ kJ/mol};$

$\Delta G_{Hess} = 32.2824 + 1175.5732 - 151.549 - (75.2864 + 1059.11 - 237.191) = 159.1 \text{ kJ/mol}$  endoergic;

$\Delta G_{HessAlbertyCH_3CH_2OH} = G_{NADH} + G_{H_3O^+} + G_{CH_3CHO} - (G_{NAD^+} + G_{CH_3CH_2OH} + G_{H_2O}) = \underline{68,02 \text{ kJ/mol}};$   
 $= 1112,534 + 22,44 + 32,282 - (1175,5 + 75,2864 - 151,549) = 68,02 \text{ kJ/mol}.$



By convention balanced **n = 2 = m** number of electrons 2e<sup>-</sup>ΔE<sup>o</sup> is expressed as E<sup>o</sup><sub>H<sub>2</sub>O</sub> of the electron donor minus E<sup>o</sup><sub>1</sub> of the electron acceptor. Because NAD<sup>+</sup> is **accepting** electrons from ethanol :

$\Delta G_{min} = \Delta G_{eq} = (E^{\circ}_{eqNernsCH_3CH_2OH} - E^{\circ}_{NAD^+}) * F * n = (-0,055 + 0,4095) * 96485 * 2 = (0,3545) * 96485 * 2 = 68,408 \text{ kJ/mol};$

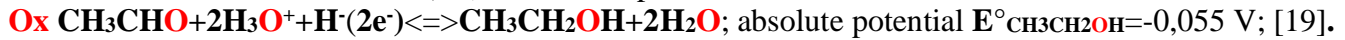
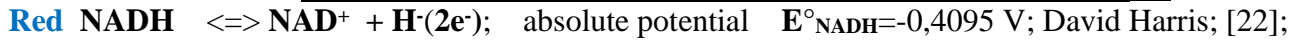
$\Delta G_{eq} = -R * T * \ln(K_{eq}); K_{eq} = \frac{[NADH] \cdot [CH_3CHO] \cdot [H_3O^+]}{[NAD^+] \cdot [CH_3CH_2OH] \cdot [H_2O]} = e^{-\frac{\Delta G_{eq}}{R * T}} = e^{-\frac{68408}{8.314 * 298.15}} = 1.036 * 10^{-12} = 10^{-11.985}$



$\Delta G_{Hess} = \Delta G^{\circ}_{CH_3CH_2OH} + \Delta G^{\circ}_{H_2O} + \Delta G^{\circ}_{NAD^+} - \Delta G^{\circ}_{H_3O} - \Delta G^{\circ}_{CH_3CHO} - \Delta G^{\circ}_{NADH} = -159.1 \text{ kJ/mol};$

$\Delta G_{Hess} = 75.2864 + 1059.11 - 237.191 - (32.2824 + 1175.5732 - 151.549) = -159.1 \text{ kJ/mol}$  endoergiska;

$\Delta G_{HessAlbertyCH_3CH_2OH} = G_{NAD^+} + G_{CH_3CH_2OH} + G_{H_2O} - (G_{NADH} + G_{H_3O^+} + G_{CH_3CHO}) = \underline{-68,02 \text{ kJ/mol}};$   
 $= 1175,5 + 75,2864 - 151,549 - (1112,534 + 22,44 + 32,282) = -68,02 \text{ kJ/mol}.$



By convention balanced **n=2=m** number of electrons 2e<sup>-</sup>ΔE<sup>o</sup> is expressed as E<sup>o</sup><sub>1</sub> of the electron donor minus E<sup>o</sup><sub>H<sub>2</sub>O</sub> of the electron acceptor. Because CH<sub>3</sub>CHO is **accepting** electrons from NADH in our example

$\Delta G_{min} = \Delta G_{eq} = (E^{\circ}_{NAD^+} - E^{\circ}_{eqNernsCH_3CH_2OH}) * F * n = (-0,4095 + 0,055) * 96485 * 2 = (-0,3545) * 96485 * 2 = -68,408 \text{ kJ/mol};$

$\Delta G_{eq} = -R * T * \ln(K_{eq}) = -68,408 \text{ kJ/mol}; K_{eq} = \frac{[NAD^+] \cdot [CH_3CH_2OH] \cdot [H_2O]}{[NADH] \cdot [CH_3CHO] \cdot [H_3O^+]} = e^{-\frac{\Delta G_{eq}}{R * T}} = e^{-\frac{-68408}{8.314 * 298.15}} = 9.65 * 10^{11} = 10^{11.985}.$

In aerobic organisms NADH oxidase with O<sub>2</sub> aqua perform ratio [NAD<sup>+</sup>]/[NADH]=10<sup>6</sup>;

$\Delta G_{Homeostāzes} = 68.408 + R * T * \ln(10^6 * 1/1 * 10^{-7.36}/55.3) = 68.408 - 86.2 = -17.8 \dots \dots \dots \text{ kJ/mol}.$

[NAD<sup>+</sup>]/[NADH]=10<sup>3</sup>;  $\Delta G_{Homeostāzes} = 68.408 - 69.08 = -0.676 \dots \dots \dots \text{ kJ/mol}.$

Equilibrium is shifted far to **reactants** as aerobic constant **K<sub>eq</sub>=10<sup>-11.985</sup>** and inverse

anaerobic constant **K<sub>eq</sub>=10<sup>11.985</sup>**. Aerobic endothermic and endoergic vitamin B<sub>3</sub> ethanol

oxidation Hess law free energy change positive  $\Delta G_{Hess}=159 \dots \dots \dots \text{ kJ/mol}$  and inverse

ethanal anaerobic reduction negative  $\Delta G_{Hess}=-159 \dots \dots \dots \text{ kJ/mol}$ , but minimises reaching

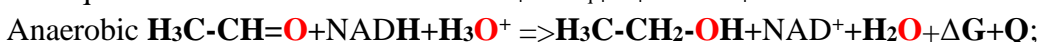
equilibrium aerobic  $\Delta G_{min} = \Delta G_{eq} = 68.4 \dots \dots \dots \text{ kJ/mol}$  and anaerobic

$\Delta G_{min} = \Delta G_{eq} = -68.4 \dots \dots \dots \text{ kJ/mol}$  reaching equilibrium mixture

constants **10<sup>-11.985</sup>=K<sub>eq</sub>** aerobic and anaerobic **10<sup>11.985</sup>=K<sub>eq</sub>**.

Prigogine attractor is free energy change absolūtā minimum  $\Delta G_{min}$  reaching

equilibrium  $\Delta G_{min} = 68.4 \dots \dots \dots \text{ kJ/mol} = |\Delta G_{eq}| < |\Delta G_{Hess}| = 159 \dots \dots \dots \text{ kJ/mol}.$



Anaerobic  $\Delta G_{eq} = \Delta E^{\circ} * F * n = -0.3545 \text{ V} * 2 \text{ mol} * 96485 \text{ C/mol} = -68.408 \dots \dots \dots \text{ kJ/mol}$  favored.

Insufficient low O<sub>2</sub> aqua concentration hypoxia to anaerobic alcohol oxidation unflavored

but ethanal reduction to ethanol favored  $[H_3CCH_2OH]/[H_3CCH=O]=1/10$

**Homeostāzes** reduction with NADH reductase enzyme as negative free energy change

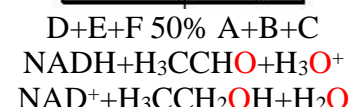
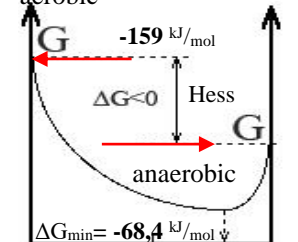
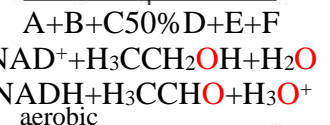
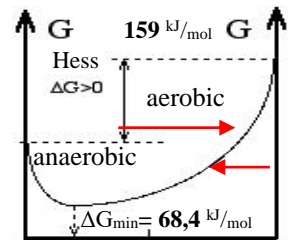
$\Delta G_{Homeostāzes} = -27.86 \dots \dots \dots \text{ kJ/mol}$

Anaerobic Homeostāzes ratio [NADH]/[NAD<sup>+</sup>]=10 over [NAD<sup>+</sup>] favors reduction:

$\Delta G_{Homeostāzes} = -68.41 + 8.3144 * 298.15 * \ln(K_{Homeostāzes}) = -68.41 + 40.54 = -27.86 \dots \dots \dots \text{ kJ/mol}$

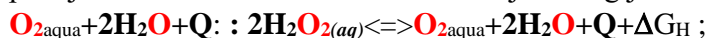
$\Delta G_{Homeostāzes} = -68.41 + 8.3144 * 298.15 * \ln\left(\frac{1}{10} \frac{1}{10} \frac{55.333}{10^{-7.36}}\right) = -27.86 \text{ kJ/mol}; K_{Homeostāzes} = \frac{[NAD^+] \cdot [CH_3CH_2OH] \cdot [H_2O]}{[NADH] \cdot [CH_3CHO] \cdot [H_3O^+]}$

$[NADH]/[NAD^+] = 1/770; \Delta G_{Homeostāzes} = 68.408 + 8.3144 * 298.15 * \ln(700/1 * 1/1 * 55.3457/10^{-7.36}) = 0.028 \text{ kJ/mol}.$





Liela ātruma protolīzes peroksīda anjonu  $\text{H}^+ + \text{HOO}^- \rightleftharpoons \text{OOH} + \text{H}^+$  sadursmes aktivācijas enerģija ir  $E_a = 79000 \text{ J/mol}$  pretēji  $\text{HOO}^- \Rightarrow \text{Fe}^{3+}$  sadursmais aktivācijas enerģija  $E_a = 29 \text{ J/mol}$  ir neliela, producējot  $\omega = 6$ ,  $\omega = 3$  taukskābes,



$\Delta G_{\text{Hess}} = \Delta G^\circ_{\text{O}_2} + 2\Delta G^\circ_{\text{H}_2\text{O}} - 2\Delta G^\circ_{\text{H}_2\text{O}_2} = 16.40 + 2*(-237.191) - (2*(-134.03)) = -189.9 \text{ kJ/mol}$  **eksoerģiska**

$\Delta G_{\text{HessAlberty}} = G^\circ_{\text{O}_2} + 2G^\circ_{\text{H}_2\text{O}} - 2G^\circ_{\text{H}_2\text{O}_2} = 303.1 + 2*(0) - (2*364.79) = -426.5/2 \text{ kJ/mol} = -213,25 \text{ kJ/mol}$  **eksoerģiska**

Viela	$\Delta H^\circ_H, \text{kJ/mol}$	$\Delta S^\circ_H, \text{J/mol/K}$	$\Delta G^\circ_H, \text{kJ/mol}$
$\text{H}_3\text{O}^+$	-285.81	-3.854	-213.275
$\text{O}_{2\text{aqua}}$	-11.715	110.876	16.4
$\text{O}_{2\text{aqua}}$	<b>-11.70</b>	<b>-94.2</b>	<b>16.40</b>
$\text{H}_2\text{O}$	-285.85	69.9565	-237.191
$\text{H}_2\text{O}$	<b>-286.65</b>	<b>-453.188</b>	<b>-151.549</b>
$\text{H}_2\text{O}_2(\text{aq})$	<b>-191.99</b>	<b>-481.688</b>	<b>-48.39</b>
$\text{H}_2\text{O}_2(\text{aq})$	-191.17	143.9	-134.03
$\text{H}_2\text{O}_2\text{l}$	-237.129	69.91	-237.129

Miščenko 1968, Himia, Leningrad

CRC 2010;

$\Delta H_{\text{Hess}} = \Delta H^\circ_{\text{O}_2} + 2\Delta H^\circ_{\text{H}_2\text{O}} - 2\Delta H^\circ_{\text{H}_2\text{O}_2} = -201.02 \dots = -201.06 \dots \text{ kJ/mol}$   
 $= -11.7 - 2*286.65 - (2*-191.99) = -201.02 \dots \text{ kJ/mol}$  **eksotermiska..**  
 $= -11.7 - 2*285.85 - (2*-191.17) = -201.06 \dots \text{ kJ/mol}$

Biochem Thermodynamic 2006 Masachusets Technology institute  
 University Alberta 1997.

2.  $\Delta S_{\text{izkļiedes}} = -\Delta H_H/T = -(-201.02)/298.15 = 674.2 \text{ J/mol/K}$  ;  $\Delta S_{\text{izkļiedes}} = -\Delta H_H/T = -(201.06)/298.15 = 674.36 \text{ J/mol/K}$  ;

$\Delta S_{\text{Hess}} = \Delta S^\circ_{\text{O}_2} + 2\Delta S^\circ_{\text{H}_2\text{O}} - 2\Delta S^\circ_{\text{H}_2\text{O}_2} = -94.2 + 2*110.876 - (2*143.9) = -37.2 \dots \text{ J/mol/K}$  ;

$\Delta S_{\text{Hess}} = \Delta S^\circ_{\text{O}_2} + 2\Delta S^\circ_{\text{H}_2\text{O}} - 2\Delta S^\circ_{\text{H}_2\text{O}_2} = 110.876 + 2*69.9565 - (2*143.9) = -37 \dots \text{ J/mol/K}$  ;

2.  $\Delta S_{\text{kopējs}} = \Delta S_H + \Delta S_{\text{izkļiedes}} = -37.2 + 674.2 = 637 \dots \text{ J/mol/K}$  ;  $\Delta S_{\text{kopējs}} = -37.011 + 674.36 = 637.35 \dots \text{ J/mol/K}$  ;

4.  $\Delta G_{\text{Hess}} = \Delta H_H - T*\Delta S_H = -201.02 - 298.15*(-0.0372) = -189.9 \dots \text{ kJ/mol}$  **eksoerģiska..... patvaļīga.....**

$\Delta G_{\text{Hess}} = \Delta H_H - T*\Delta S_H = -201.06 - 298.15*(-0.037) = -190 \dots \text{ kJ/mol}$  ;

$T*\Delta S_{\text{kopējs}} = 0.637*298.15 = 189.9 \dots \text{ kJ/mol}$  ;  $T*\Delta S_{\text{kopējs}} = 0.63735*298.15 = 190 \dots \text{ kJ/mol}$  ;

$[\text{H}_2\text{O}_2] = 1$  ;  $10^{(-10)}$  M biokīmijas koncentrācijas  $[\text{O}_{2\text{aqua}}] = 6*10^{-5}$  M,  $[\text{H}_3\text{O}^+] = 10^{-7.36}$  M,  $[\text{H}_2\text{O}] = 55,3$  M.

**Red**  $\text{H}_2\text{O}_2 + 2\text{H}_2\text{O} = \text{O}_2 + 2\text{H}_3\text{O}^+ + 2\text{e}^-$  ;  $E^\circ_{\text{H}_2\text{O}_2} = 0,4495$  V **absolūtais** standarta potenciāls ;  $E_{\text{Red}} = E^\circ_{\text{H}_2\text{O}_2} + 0,0591/2*$

$\lg([\text{O}_{2\text{aqua}}]*[\text{H}_3\text{O}^+]^2/[\text{H}_2\text{O}_2]/[\text{H}_2\text{O}]^2) = 0,4495 + 0,0591/2*\lg(6*10^{(-5)}*10^{(-7.36*2)}/10^{(-10)}/55,3^2) = 0,08227$  V

$E_{\text{Red}} = E^\circ_{\text{H}_2\text{O}_2} + 0,0591/2*\lg([\text{O}_{2\text{aqua}}]*[\text{H}_3\text{O}^+]^2/[\text{H}_2\text{O}_2]/[\text{H}_2\text{O}]^2) = 0,4495 + 0,0591/2*\lg(6*10^{(-5)}*10^{(-7.36*2)}/1/55,3^2) = -0,2132$  V

**Ox**  $\text{H}_2\text{O}_2 + 2\text{H}_3\text{O}^+ + 2\text{e}^- = 4\text{H}_2\text{O}$  ;  $-E^\circ_{\text{OxH}_2\text{O}_2} = -1,6855$  V **absolūtais inversais** standarta potenciāls ;

$-E_{\text{Ox}} = -E^\circ_{\text{H}_2\text{O}_2\text{Ox}} + 0,0591/2*\lg([\text{H}_2\text{O}]^4/[\text{H}_2\text{O}_2]/[\text{H}_3\text{O}^+]^2) = -1,6855 + 0,0591/2*\lg(55,3^4/10^{(-7.36*2)}/10^{(-10)}) = -0,749$  V ;

$-E_{\text{Ox}} = -E^\circ_{\text{H}_2\text{O}_2\text{Ox}} + 0,0591/2*\lg([\text{H}_2\text{O}_2]*[\text{H}_3\text{O}^+]^2/[\text{H}_2\text{O}]^4) = -1,6855 + 0,0591/2*\lg(1*10^{(-7.36*2)}/55,3^4) = -2,3265$  V

$[\text{H}_2\text{O}_2] = 1$  M ;  $[\text{H}_2\text{O}_2] = 10^{(-10)}$  M ; koncentrācijas  $2\text{H}_2\text{O}_{2\text{aq}} \Rightarrow \text{O}_{2\text{aqua}} + 2\text{H}_2\text{O}$  ;

$[\text{H}_2\text{O}_2] = 10^{(-10)}$  M ;  $\Delta G_{\text{eqBioChem}} = (E^\circ_{\text{Red}} - E^\circ_{\text{Ox}})*F*n = (0,08227 - 0,749)*96485*2 = (-1,236)*96485*2 = -238,5 \text{ kJ/mol}$  ;

$[\text{H}_2\text{O}_2] = 1$  M ;  $\Delta G_{\text{eqBioChem}} = (E_{\text{Red}} - E_{\text{Ox}})*F*n = (-0,2132 - 2,3265)*96485*2 = (-2,5397)*96485*2 = -490,1 \text{ kJ/mol}$  ;

$\Delta G_{\text{Alberty}} = G_{\text{O}_2\text{BioChem}_\text{arterijā}} + 2*G_{\text{H}_2\text{O}\text{BioChemistry}} - 2*G_{\text{H}_2\text{O}_2} = 78,08 + 2*85,64 - 2*364,79 = -480,22 \text{ kJ/mol}$  ;

$2\text{H}_2\text{O}_2(\text{aq}) \Rightarrow \text{O}_{2\text{aqua}} + 2\text{H}_2\text{O} + \text{Q} + \Delta G$  ; Homeostāzes produktu aktivēšana, hidroksonija un peroksīda anjonu:

$G_{\text{H}_2\text{O}_2} = 364,8 \text{ kJ/mol}$  ;  $G_{\text{H}_3\text{O}^+} + G_{\text{HOO}^-} = 22,44 + 418,32 = 440,76 \text{ kJ/mol}$  absolūtās brīvās enerģijas attiecinātas uz ūdens un  $\text{CO}_2\text{gas}$

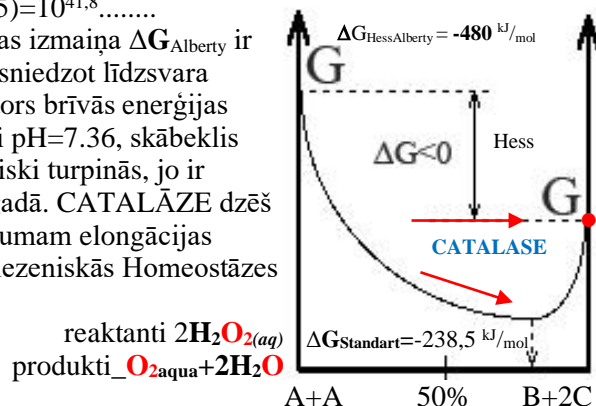
nulles  $G_{\text{H}_2\text{O}} = G_{\text{CO}_2\text{gas}} = 0 \text{ kJ/mol}$  vērtību:

$\Delta G_{\text{eqStandard}} = (E^\circ_{\text{H}_2\text{O}_2} - E^\circ_{\text{H}_2\text{O}_2\text{Ox}})*F*n = (0,4495 - 1,6855)*96485*2 = (-1,1845)*96485*2 = -238,5 \dots \text{ kJ/mol}$  ;

$\Delta G_{\text{HessAlberty}} = G_{\text{O}_2} + 2G_{\text{H}_2\text{O}} - 2G_{\text{H}_2\text{O}_2} = 330 + 2*(0) - (2*284) = -238 \text{ kJ/mol}$  ; **Alberty**

$K_{\text{eqStandard}} = K_{\text{H}_2\text{O}_2} = \exp(-\Delta G_{\text{eq}}/R/T) = \exp(238500/8.3144/298.15) = 10^{41.8} \dots$

Eksotermiska un eksoerģiska  $\text{H}_2\text{O}_2(\text{aq})$  dismutēšanas Hesa brīvās enerģijas izmaiņa  $\Delta G_{\text{Alberty}}$  ir negatīva  $-480 \dots \text{ kJ/mol}$ , bet minimizējas  $\Delta G_{\text{eqStandard}} = -238,5 \dots \text{ kJ/mol}$  sasniedzot līdzsvara maisījuma konstanti  $K_{\text{eq}} = 10^{41.8} \dots$ . Lešateljē princips ir Prigožina atraktors brīvās enerģijas izmaiņas minimuma  $\Delta G_{\text{min}}$  sasniegšana. Liela ātruma protolīzes atraktori pH=7.36, skābeklis 20.95% gaisā atrodas līdzsvara stāvoklī, kamēr Homeostāze neatgriezeniski turpinās, jo ir nelīdzsvara stāvoklis. Prigožina atraktors Nobela Prēmija ķīmijā 1977. gadā. CATALĀZE dzēs peroksīda molekulas  $\text{H}_2\text{O}_2$  līdz 100%  $\omega = 6$ ,  $\omega = 3$  taukskābju C20:4 iznākumam elongācijas sintēzē peroksisomās. CATALĀZES reaktivitāte ir nepieciešams neatgriezeniskās Homeostāzes Brauna molekulārais dzinējs evolūcijai un izdzīvošanai.



reaktanti  $2\text{H}_2\text{O}_2(\text{aq})$   
 produkti  $\text{O}_{2\text{aqua}} + 2\text{H}_2\text{O}$

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