

Sēra savienojumu šķīšanas, protolīzes un reducēšanas-oksīdēšanas Prigožina absolūtās enerģijas atraktori.

Viela	$\Delta H^\circ_{\text{H}}$ kJ/mol	$\Delta S^\circ_{\text{H}}$ J/mol/K	$\Delta G^\circ_{\text{H}}$ kJ/mol
$\text{H}_2\text{S}^{\text{gas}}$	formation	$\Delta G^\circ -33,4$	55,7436
$\text{H}_2\text{S}^{\text{gas}}$	Solubility	promote	69,073
$\text{H}_2\text{S}^{\text{gas}}$	-20,6	205,81	-33,4
$\text{H}_2\text{S}_{\text{aq}}$	-22,9596	-256,064	53,3896
$\text{H}_2\text{S}_{\text{aq}}$	$E^\circ_{\text{S}^2/\text{H}_2\text{S}_{\text{aq}}}$	-0,025735 V	53,3896
$\text{H}_2\text{S}_{\text{aq}}$	$\text{S} + 2\text{H}(\text{Pt}) =$	$\text{H}_2\text{S}_{\text{aq}}$	53,3866
HS^-	-16,3	67	12,5
$\text{HS}^- \text{ Ge-}$	formation	12,5	31,69
HS^-	$E^\circ_{\text{S}^2/\text{S}_2}$	-0,8517V	90,5336
HS^-	$\text{pK}_{\text{a}1}=7,05$	favored	81,138
HS^-	$\text{pK}_{\text{a}2}=19$	-	92,63
$\text{S}_{\text{rhom}}^{\text{bic}}$	formation	-	3,5436
$\text{S}_{\text{rhom}}^{\text{bic}}$	$E^\circ_{\text{S}^2/\text{H}_2\text{S}_{\text{aq}}}$	-0,025735 V	3,5436
S^{2-}	33,1	-14,6	85,8
$\text{S}^{2-} \text{ Ge-}$	formation	85,8	2*34,1432
S^{2-}	$E^\circ_{\text{S}^2/\text{S}_2}$	-0,79853V	157,63

$\text{GH}_2\text{S}^{\text{gas}} = 85,6 \text{ kJ/mol}$; $\text{GH}_2\text{S}_{\text{aq}} = 53,3896 \text{ kJ/mol}$; $\text{GS}_{\text{rhom}}^{\text{bic}} = 3,5436 \text{ kJ/mol}$;
 favored $\text{GH}_2\text{S}^{\text{gas}} = \Delta G^\circ_{\text{H}_2\text{S}^{\text{gas}}} + (\text{GS}_{\text{rhom}}^{\text{bic}} + \text{GH}_2) = 55,7436 \text{ kJ/mol}$;
 $\text{GH}_2\text{S}^{\text{gas}} = \text{GH}_2\text{S}_{\text{aq}} + (\Delta G_{\text{eq}} + \text{GH}_2\text{O}) = 84,343 + (15,27 + 0) = 69,073 \text{ kJ/mol}$;
 [1] $\Delta \text{GH}_2\text{S}^{\text{gas}} = \Delta H_{\text{H}} - T \cdot \Delta S_{\text{H}} = -20,6 - 298,15 \cdot 0,20581 = -81,96 \text{ kJ/mol}$;
 2006, Massachusetts Technology Inst. pH=7,36 Alberty [8]
 $\text{GH}_2\text{S}_{\text{aq}} = \text{GS}_{\text{rhom}}^{\text{bic}} + 2\text{GH}_3\text{O} + (-\Delta G_{\text{eqH}_2\text{S}_{\text{aq}}} + 2\text{GH}_2\text{O}) = 53,3896 \text{ kJ/mol}$;
 $\text{GH}_2\text{S}_{\text{aq}} = \Delta G_{\text{HessH}_2\text{S}} + (2\text{GH}(\text{Pt}) + \text{GS}_{\text{rhom}}^{\text{bic}}) = 53,3866 \text{ kJ/mol}$;
 [1] $\Delta \text{GH}_{\text{S}} = \Delta H_{\text{H}} - T \cdot \Delta S_{\text{H}} = -16,3 - 298,15 \cdot 0,067 = -36,276 \text{ kJ/mol}$;
 $\text{Ge-} = \text{GH}_{\text{S}} - (\text{GS}_{\text{r}} + 0,5\text{GH}_2 + \Delta G^\circ_{\text{HS}}) = 31,69 \text{ kJ/mol}$;
 $\text{pK}_{\text{a}2} = 19$ $\text{GH}_{\text{S-aq}} = \text{GS}_{\text{rhom}}^{\text{bic}} + 2\text{GH}_2\text{O} - (\Delta G_{\text{eqHS-aq}} + \text{GOH}) = 90,5336 \text{ kJ/mol}$;
 favored $\text{GH}_{\text{S}} = \Delta G_{\text{eq}} - \text{GH}_3\text{O} + (\text{GH}_2\text{S} + \text{GH}_2\text{O}) = 81,138 \text{ kJ/mol}$;
 $\text{GH}_{\text{S}} = \text{GS}_2 - \text{GH}_3\text{O} - (\Delta G_{\text{eq}} + \text{GH}_2\text{O}) = 92,65 \text{ kJ/mol}$;
 $\text{GS}_{\text{rhom}}^{\text{bic}} = \text{GH}_2\text{S}^{\text{gas}} - (\Delta G_{\text{HessH}_2\text{S}} + \text{GH}_2) = 3,5436 \text{ kJ/mol}$;
 favored $\text{GS}_{\text{rhom}}^{\text{bic}} = \Delta G_{\text{eqH}_2\text{S}_{\text{aq}}} - 2\text{GH}_3\text{O} + (\text{GH}_2\text{S}_{\text{aq}} + 2\text{GH}_2\text{O}) = 3,544 \text{ kJ/mol}$;
 [1] $\Delta \text{GH}_{\text{S}} = \Delta H_{\text{H}} - T \cdot \Delta S_{\text{H}} = 33,1 - 298,15 \cdot 0,0146 = -36,276 \text{ kJ/mol}$;
 $2\text{Ge-} = \text{GS}_2 - (\text{GS}_{\text{r}} + \Delta G^\circ_{\text{S}_2}) = 157,63 - (3,5436 + 85,8) = 2*34,1432 \text{ kJ/mol}$;
 $\text{GS}_2\text{-aq} = \text{GS}_{\text{rhom}}^{\text{bic}} + \text{GH}_2\text{O} - (\Delta G_{\text{eqS}_2\text{-aq}}) = 157,63 \text{ kJ/mol}$;

Veidošanās no elementiem $\text{S}_{\text{rhom}}^{\text{bic}} + \text{H}_2\text{S}^{\text{gas}} = \text{H}_2\text{S}_{\text{aq}}$ uzrāda enerģijas saturu $\text{GH}_2\text{S}^{\text{gas}} = 55,7436 \text{ kJ/mol}$;

Enerģijas saturs ir $\text{GH}_2\text{S}^{\text{gas}} = \Delta G^\circ_{\text{H}_2\text{S}^{\text{gas}}} + (\text{GS}_{\text{rhom}}^{\text{bic}} + \text{GH}_2) = -33,4 + (3,5436 + 85,6) = 55,7436 \text{ kJ/mol}$. [1,8]

Enerģijas saturs ir $\text{GS}_{\text{rhom}}^{\text{bic}} = \text{GH}_2\text{S}^{\text{gas}} - (\Delta G^\circ_{\text{H}_2\text{S}^{\text{gas}}} + \text{GH}_2) = 55,7436 - (-33,4 + 85,6) = 3,5436 \text{ kJ/mol}$. [1,8]

Formation $\text{S}_{\text{rhom}}^{\text{bic}} + 0,5\text{H}_2\text{S}^{\text{gas}} + \text{e}^- = \text{HS}^-$;

$$\Delta G^\circ_{\text{HS}} = \text{GH}_{\text{S}} - (\text{GS}_{\text{r}} + 0,5\text{GH}_2 + \text{Ge-}) = 90,5336 - (3,5436 + 0,5 \cdot 85,6 + \text{Ge-}) = 12,5 \text{ kJ/mol}.$$

$$\text{Ge-} = \text{GH}_{\text{S}} - (\text{GS}_{\text{r}} + 0,5\text{GH}_2 + \Delta G^\circ_{\text{HS}}) = 90,5336 - (3,5436 + 0,5 \cdot 85,6 + 12,5) = 31,69 \text{ kJ/mol}.$$

$$\text{GH}_{\text{S}} = \Delta G^\circ_{\text{HS}} + (\text{GS}_{\text{r}} + 0,5\text{GH}_2 + \text{Ge-}) = 12,5 + (3,5436 + 0,5 \cdot 85,6 + 31,69) = 90,5336 \text{ kJ/mol}.$$

Formation $\text{S}_{\text{rhom}}^{\text{bic}} + 2\text{e}^- = \text{S}^{2-}$; $\Delta G^\circ_{\text{S}_2} = \text{GS}_2 - (\text{GS}_{\text{r}} + 2\text{Ge-}) = 157,63 - (3,5436 + 2\text{Ge-}) = 85,8 \text{ kJ/mol}$.

$$2\text{Ge-} = \text{GS}_2 - (\text{GS}_{\text{r}} + \Delta G^\circ_{\text{S}_2}) = 157,63 - (3,5436 + 85,8) = 2*34,1432 \text{ kJ/mol}.$$

$$\text{GS}_2 = \Delta G^\circ_{\text{S}_2} + (\text{GS}_{\text{r}} + 2\text{Ge-}) = 85,8 + (3,5436 + 2*34,1432) = 157,63 \text{ kJ/mol}.$$

Šķīdības $\text{H}_2\text{S}^{\text{gas}} + \text{H}_2\text{O} = \text{H}_2\text{S}_{\text{aq}}$ 3,98 g/L 20° C [30] $\text{M}_{\text{H}_2\text{S}} = 34,08 \text{ g/mol}$ produkts $\text{K}_{\text{sp}} = [\text{H}_2\text{S}_{\text{aq}}] = 3,98/34,08 = 0,11678 \text{ M}$
 līdzsvara konstante ir $\text{K}_{\text{eq}} = \text{K}_{\text{sp}}/[\text{H}_2\text{O}] = 0,116784/55,3 = 0,0021118$ ar endoergonisku brīvās enerģijas izmaiņu
 pozitīvu $\Delta G_{\text{eq}} = -R \cdot T \cdot \ln(\text{K}_{\text{eq}}) = -8,3144 \cdot 298,15 \cdot \ln(0,0021118) = \text{GH}_2\text{S}_{\text{aq}} - (\text{GH}_2\text{S}^{\text{gas}} + \text{GH}_2\text{O}) = 15,27 \text{ kJ/mol}$.

$$\Delta G_{\text{eq}} = \text{GH}_2\text{S}_{\text{aq}} - (\text{GH}_2\text{S}^{\text{gas}} + \text{GH}_2\text{O}) = 84,343 - (69,073 + 0) = 15,27 \text{ kJ/mol}.$$

Brīvās enerģijas saturs molā sērūdeņraža ir $\text{GH}_2\text{S}^{\text{gas}} = \text{GH}_2\text{S}_{\text{aq}} + (\Delta G_{\text{eq}} + \text{GH}_2\text{O}) = 84,343 - (15,27 + 0) = 69,073 \text{ kJ/mol}$.

$\text{S}^{2-} = \text{S}_{\text{rhom}}^{\text{bic}} + \text{H}_2\text{O} + 2\text{e}^-$; Classic standarta potenciāls $E^\circ_{\text{Classic}} = -0,4763 \text{ V}$ [1], plus ūdens uzskaitē
 $-0,0591/2 \cdot \log([\text{H}_2\text{O}]^1) = -0,0515$ un saistītā summa $\Delta E^\circ = +0,10166 - 0,37239$ izteiksmē absolūtais potenciāls ir

$$E^\circ_{\text{S}^2/\text{S}_2} = E^\circ_{\text{Classic}} - 0,0591/2 \cdot \log([\text{H}_2\text{O}]^1) + \Delta E^\circ = -0,4763 - 0,0515 + 0,10166 - 0,37239 = -0,79853 \text{ V};$$

$$\Delta G_{\text{eqS}_2} = E^\circ_{\text{S}_2} \cdot F \cdot n = -0,79853 \cdot 96485 \cdot 2 = -154,09 \text{ kJ/mol}.$$
 $\text{GS}_{\text{rhom}}^{\text{bic}} = 3,5436 \text{ kJ/mol}$;

$$\Delta G_{\text{eqS}_2\text{-aq}} = \text{GS}_{\text{rhom}}^{\text{bic}} + \text{GH}_2\text{O} + 2\text{Ge-} - (\text{GS}_2\text{-aq}) = 3,5436 + 0 + 2*0 - (157,6336) = -154,09 \text{ kJ/mol};$$

$$2\text{Ge-} = \Delta G_{\text{eqS}_2\text{-aq}} - \text{GS}_{\text{rhom}}^{\text{bic}} - \text{GH}_2\text{O} + (\text{GS}_2\text{-aq}) = -154,09 - 3,5436 - 0 + (157,6336) = 0 \text{ kJ/mol};$$

$$\text{GS}_2\text{-aq} = \text{GS}_{\text{rhom}}^{\text{bic}} + \text{GH}_2\text{O} + 2\text{Ge-} - (\Delta G_{\text{eqS}_2\text{-aq}}) = 3,5436 + 0 + 2*0 - (-154,09) = 157,63 \text{ kJ/mol};$$

$\text{HS}^- + \text{OH}^- = \text{S}_{\text{rhom}}^{\text{bic}} + 2\text{H}_2\text{O} + 2\text{e}^-$; Classic standarta potenciāls $E^\circ_{\text{Classic}} = -0,478 \text{ V}$ [1], plus ūdens uzskaitē
 $-0,0591/2 \cdot \log([\text{H}_2\text{O}]^2) = -0,103$ un saistītā summa $\Delta E^\circ = +0,10166 - 0,37239$ izteiksmē absolūtais potenciāls ir

$$E^\circ_{\text{S}^2/\text{HS}} = E^\circ_{\text{Classic}} - 0,0591/2 \cdot \log([\text{H}_2\text{O}]^2) + \Delta E^\circ = -0,478 - 0,103 + 0,10166 - 0,37239 = -0,8517 \text{ V};$$

$$\Delta G_{\text{eqHS}} = E^\circ_{\text{HS}} \cdot F \cdot n = -0,8517 \cdot 96485 \cdot 2 = -164,35 \text{ kJ/mol};$$

$$\Delta G_{\text{eqHS-aq}} = \text{GS}_{\text{rhom}}^{\text{bic}} + 2\text{GH}_2\text{O} + 2\text{Ge-} - (\text{GH}_{\text{S-aq}} + \text{GOH}) = 3,5436 + 2*0 + 2*0 - (90,5336 + 77,36) = -164,35 \text{ kJ/mol};$$

$$\text{GH}_{\text{S-aq}} = \text{GS}_{\text{rhom}}^{\text{bic}} + 2\text{GH}_2\text{O} + 2\text{Ge-} - (\Delta G_{\text{eqHS-aq}} + \text{GOH}) = 3,5436 + 2*0 + 2*0 - (-164,35 + 77,36) = 90,5336 \text{ kJ/mol};$$

$$2\text{Ge-} = \Delta G_{\text{eqHS-aq}} - \text{GS}_{\text{rhom}}^{\text{bic}} - 2\text{GH}_2\text{O} + (\text{GH}_{\text{S-aq}} + \text{GOH}) = -164,35 - 3,5436 - 2*0 + (90,5336 + 77,36) = 0 \text{ kJ/mol};$$

$\text{H}_2\text{S}_{\text{aq}} + 2\text{H}_2\text{O} = \text{S}_{\text{rhom}}^{\text{bic}} + 2\text{H}_3\text{O}^+ + 2\text{e}^-$; Classic standarta potenciāls $E^\circ_{\text{Classic}} = 0,142 \text{ V}$ [1], plus ūdens uzskaitē
 $-0,0591/2 \cdot \log(1/[\text{H}_2\text{O}]^2) = 0,103$ un saistītā summa $\Delta E^\circ = +0,10166 - 0,37239$ izteiksmē absolūtais potenciāls ir

$$E^\circ_{\text{S}^2/\text{H}_2\text{S}} = E^\circ_{\text{Classic}} - 0,0591/2 \cdot \log(1/[\text{H}_2\text{O}]^2) + \Delta E^\circ = 0,142 + 0,103 + 0,10166 - 0,37239 = -0,025735 \text{ V};$$

$$\Delta G_{\text{eqH}_2\text{S}} = E^\circ_{\text{H}_2\text{S}} \cdot F \cdot n = -0,025735 \cdot 96485 \cdot 2 = -4,966 \text{ kJ/mol};$$

$$\Delta G_{\text{eqH}_2\text{S}_{\text{aq}}} = \text{GS}_{\text{rhom}}^{\text{bic}} + 2\text{GH}_3\text{O} + 2\text{Ge-} - (\text{GH}_2\text{S}_{\text{aq}} + 2\text{GH}_2\text{O}) = 3,5436 + 2*22,44 + 2*0 - (53,3896 + 2*0) = -4,966 \text{ kJ/mol};$$

$$\text{GS}_{\text{rhom}}^{\text{bic}} = \Delta G_{\text{eqH}_2\text{S}_{\text{aq}}} - 2\text{GH}_3\text{O} + 2\text{Ge-} + (\text{GH}_2\text{S}_{\text{aq}} + 2\text{GH}_2\text{O}) = -4,966 - 2*22,44 - 2*0 + (53,3896 + 2*0) = 3,5436 \text{ kJ/mol};$$
 favored

$$G_{H_2S_{aq}} = G_{S_{rubic}} + 2G_{H_3O^+} + 2G_{e^-} - (\Delta G_{eqH_2S_{aq}} + 2G_{H_2O}) = 3,5436 + 2 \cdot 22,44 + 2 \cdot 0 - (-4,966 + 2 \cdot 0) = 53,3896 \text{ kJ/mol};$$

$$2G_{e^-} = \Delta G_{eqH_2S_{aq}} - G_{S_{rubic}} - 2G_{H_3O^+} + (G_{H_2S_{aq}} + 2G_{H_2O}) = -4,966 - 3,5436 - 2 \cdot 22,44 + (53,3896 + 2 \cdot 0) = 2 \cdot 0 \text{ kJ/mol};$$

$$[1] \text{ p}K_{a1} = 7,05; \text{ p}K_{a2} = 19;$$

$$\text{p}K_{a1} = 7,05 \quad H_2S + H_2O = HS^- + H_3O^+; K_{eq1} = K_{a1}/[H_2O] = 10^{-(7,05)}/55,3 = 0,000000001612;$$

$$\Delta G_{eq} = -R \cdot T \cdot \ln(K_{eq}) = -8,3144 \cdot 298,15 \cdot \ln(0,000000001612) = G_{HS^-} + G_{H_3O^+} - (G_{H_2S} + G_{H_2O}) = 50,188 \text{ kJ/mol};$$

$$\Delta G_{eq} = G_{HS^-} + G_{H_3O^+} - (G_{H_2S} + G_{H_2O}) = 81,138 + 22,44 - (53,3896 + 0) = 50,188 \text{ kJ/mol};$$

$$G_{HS^-} = \Delta G_{eq} - G_{H_3O^+} + (G_{H_2S} + G_{H_2O}) = 50,188 - 22,44 + (53,3896 + 0) = 81,138 \text{ kJ/mol};$$

$$\text{p}K_{a2} = 19 \quad HS^- + H_2O = S^{2-} + H_3O^+; K_{eq1} = K_{a1}/[H_2O] = 10^{-(19)}/55,3 = 10^{-(20,74)};$$

$$\Delta G_{eq} = -R \cdot T \cdot \ln(K_{eq}) = -8,3144 \cdot 298,15 \cdot \ln(10^{-(20,74)}) = G_{S^{2-}} + G_{H_3O^+} - (G_{HS^-} + G_{H_2O}) = 118,40 \text{ kJ/mol};$$

$$\Delta G_{eq} = G_{S^{2-}} + G_{H_3O^+} - (G_{HS^-} + G_{H_2O}) = 186,4936 + 22,44 - (90,5336 + 0) = 118,40 \text{ kJ/mol};$$

$$G_{S^{2-}} = \Delta G_{eq} - G_{H_3O^+} + (G_{HS^-} + G_{H_2O}) = 118,40 - 22,44 + (90,5336 + 0) = 186,4936 \text{ kJ/mol};$$

$$G_{HS^-} = G_{S^{2-}} + G_{H_3O^+} - (\Delta G_{eq} + G_{H_2O}) = 186,4936 + 22,44 - (118,40 + 0) = 90,5336 \text{ kJ/mol};$$

$$\text{Sēra reducēšana inversais potenciāls: } S_{rubic} + 2H_3O^+ + 2e^- = H_2S_{aq} + 2H_2O; -E^\circ_s = 0,025735 \text{ V};$$

$$2H(Pt) + 2H_2O = 2H_3O^+ + 2e^-; E^\circ_H = -0,27073 \text{ V}; \text{ sumārā reakcija } S_{rubic} + 2H(Pt) = H_2S_{aq};$$

$$\Delta G_{eq} = (E^\circ_H - E^\circ_s) \cdot F \cdot n = (-0,27073 + 0,025735) \cdot 96485 \cdot 2 = -0,244995 \cdot 96485 \cdot 2 = -47,277 \text{ kJ/mol};$$

$$\Delta G_{HessH_2S} = G_{H_2S_{aq}} - (2G_{H(Pt)} + G_{S_{rubic}}) = 53,3866 - (2 \cdot 48,56 + 3,5436) = -47,277 \text{ kJ/mol};$$

$$G_{H_2S_{aq}} = \Delta G_{HessH_2S} + (2G_{H(Pt)} + G_{S_{rubic}}) = -47,277 + (2 \cdot 48,56 + 3,5436) = 53,3866 \text{ kJ/mol};$$

$$\text{Albertija [8] un CRC [1] dati: } G_{H_2}^{gas} = 85,6 \text{ kJ/mol}, G_{H_2S_{aq}} = 53,3866 \text{ kJ/mol [8] un } \Delta G^\circ_{H_2O} = -237,191 \text{ kJ/mol},$$

$$\Delta G^\circ_{H_2S}^{gas} = -81,98 \text{ kJ/mol [1] ļauj aprēķināt vielu absolūtās vērtības brīvās enerģijas saturam } G_{S_{rubic}} = 3,5436 \text{ kJ/mol},$$

$$G_{O_2}^{gas} = 303,1 \text{ kJ/mol} \text{ utt. attiecībā pret ūdeni un oglekļa dioksīda gāzes nulli } G_{H_2O} = G_{CO_2}^{gas} = G_{e^-} = 0 \text{ kJ/mol} \text{ skalā.}$$

$$[1] \quad H_2SO_4 \text{ veidošanās no brīviem elementiem sērskābei un sulfātiem: } S_{rubic} + 2O_2^{gas} + H_2^{gas} = H_2SO_4;$$

$$\Delta G^\circ_{H_2SO_4 \text{ Form}} = G_{H_2SO_4} - (G_{S_{rubic}} + 2G_{O_2} + G_{H_2}^{gas}) = -690,0 \text{ kJ/mol}; \text{ Saturs molā sērskābes ir}$$

$$G_{H_2SO_4} = \Delta G^\circ_{H_2SO_4 \text{ Form}} + (G_{S_{rubic}} + 2G_{O_2} + G_{H_2}^{gas}) = -690,0 + (3,5436 + 2 \cdot 303,1 + 85,6) = 5,3436 \text{ kJ/mol}.$$

$$[1] \quad SO_3 \text{ veidošanās no elementiem } S_{rubic} + 1,5O_2^{gas} = SO_3; \Delta G^\circ_{SO_3 \text{ Form}} = G_{SO_3} - (3,5436 + 1,5 \cdot 303,1) = -373,8 \text{ kJ/mol};$$

$$G_{SO_3} = \Delta G^\circ_{SO_3 \text{ Form}} + (G_{S_{rubic}} + 1,5G_{O_2}) = -373,8 + (3,5436 + 1,5 \cdot 303,1) = 84,3936 \text{ kJ/mol};$$

$$100\% \text{ sērskābes veidošanās, oleumam šķīstot ūdenī, ir eksoergoniska } SO_3 + H_2O = H_2SO_4;$$

$$\Delta G^\circ_{SO_3 + H_2O} = G_{H_2SO_4} - (G_{SO_3} + G_{H_2O}) = 5,1436 - (84,2436 + 0) = -79,1 \text{ kJ/mol};$$

$$\text{Protolīzes } \text{p}K_{a1} = -2,8 \text{ līdzsvaru } H_2SO_4 + H_2O = HSO_4^- + H_3O^+ \text{ molu daļās aprēķina dalot skābes konstanti } K_{a1} \text{ ar}$$

$$\text{ūdens koncentrāciju } [H_2O] = 55,3 \text{ M } K_{eq1} = K_{a1}/[H_2O] = 10^{-(2,8)}/55,3 = 11,4097. \text{ Prigožina atraktors un Hesa aprēķins}$$

$$\text{ir vienādi eksoergonisks: } \Delta G_{eqH_2SO_4} = -R \cdot T \cdot \ln(K_{eq}) = -8,3144 \cdot 298,15 \cdot \ln(11,4097) = -6,0349 \text{ kJ/mol};$$

$$\Delta G_{eqH_2SO_4} = G_{HSO_4^-} + G_{H_3O^+} - (G_{H_2SO_4} + G_{H_2O}) = 27,5836 + 22,44 - (56,0586 + 0) = -6,0349 \text{ kJ/mol};$$

$$G_{HSO_4^-} = \Delta G_{eqH_2SO_4} - G_{H_3O^+} + (G_{H_2SO_4} + G_{H_2O}) = -6,0349 - 22,44 + (56,0586 + 0) = 27,5835 \text{ kJ/mol};$$

$$H_2SO_4 \text{ molā ir } G_{H_2SO_4} = G_{HSO_4^-} + G_{H_3O^+} - (\Delta G_{eqH_2SO_4} + G_{H_2O}) = 27,5835 + 22,44 - (-6,0349 + 0) = 56,0585 \text{ kJ/mol}.$$

$$\text{Protolīzes } \text{p}K_{a2} = 1,99 \quad HSO_4^- + H_2O = SO_4^{2-} + H_3O^+$$

$$K_{eq2} = K_{a2}/[H_2O] = 10^{-(1,99)}/55,3 = 0,00018504 \text{ enerģijas izmaiņa ir}$$

$$\Delta G_{eqHSO_4} = -R \cdot T \cdot \ln(K_{eq2}) = -8,3144 \cdot 298,15 \cdot \ln(0,00018504) = 21,3069 \text{ kJ/mol. Izmaiņa Hesa izteiksmē}$$

$$\Delta G_{eqHSO_4} = G_{SO_4^{2-}} + G_{H_3O^+} - (G_{HSO_4^-} + G_{H_2O}) = 26,4509 + 22,44 - (27,584 + 0) = 21,3064 \text{ kJ/mol}$$

$$G_{SO_4^{2-}} = G_{SO_4^{2-}} + G_{H_3O^+} - (\Delta G_{eqHSO_4} + G_{H_2O}) = 26,4509 + 22,44 - (21,3069 + 0) = 27,584 \text{ kJ/mol};$$

$$SO_4^{2-} \text{ anjona molā ir } G_{SO_4^{2-}} = \Delta G_{eqHSO_4} - G_{H_3O^+} + (G_{HSO_4^-} + G_{H_2O}) = 21,3069 - 22,44 + (27,584 + 0) = 26,4509 \text{ kJ/mol};$$

$$[1] \text{ Formation } S_{rubic} + 2O_2^{gas} + 0,5H_2^{gas} + e^- = HSO_4^-; G_e = 119,5401 \text{ kJ/mol}; G_{HSO_4^-} = 27,5837 \text{ kJ/mol}; \text{ p}K_{a2} = 1,99;$$

$$\Delta G^\circ_{HSO_4} = G_{HSO_4^-} - (G_{S_{rubic}} + 2G_{O_2} + 0,5G_{H_2}^{gas} + G_e) = 27,5837 - (3,5436 + 2 \cdot 303,1 + 0,5 \cdot 85,6 + 119,5401) = -744,5 \text{ kJ/mol};$$

$$G_{HSO_4^-} = \Delta G^\circ_{HSO_4} + (G_{S_{rubic}} + 2G_{O_2} + 0,5G_{H_2}^{gas} + G_e) = -744,5 + (3,5436 + 2 \cdot 303,1 + 0,5 \cdot 85,6 + 119,54) = 27,5837 \text{ kJ/mol};$$

$$G_e = G_{HSO_4^-} - (G_{S_{rubic}} + 2G_{O_2} + 0,5G_{H_2}^{gas} + \Delta G^\circ_{HSO_4}) = 27,5837 - (3,5436 + 2 \cdot 303,1 + 0,5 \cdot 85,6 - 744,5) = 119,54 \text{ kJ/mol};$$

$$[1] \text{ Formation } S_{rubic} + 2O_2^{gas} + 2e^- = SO_4^{2-};$$

$$\Delta G^\circ_{SO_4^{2-}} = G_{SO_4^{2-}} - (G_{S_{rubic}} + 2G_{O_2} + 2G_e) = 26,44977 - (3,5436 + 2 \cdot 303,1 + 2 \cdot 80,603) = -744,5 \text{ kJ/mol};$$

$$2G_e = G_{SO_4^{2-}} - (G_{S_{rubic}} + 2G_{O_2} + \Delta G^\circ_{SO_4^{2-}}) = 26,44977 - (3,5436 + 2 \cdot 303,1 - 744,5) = 161,20617 = 2 \cdot 80,603 \text{ kJ/mol};$$

$$\text{https://en.wikipedia.org/wiki/Sulfur_dioxide}$$

$$\text{Šķīdības konstantes molu daļās } K_{eq} = K_{sp}/[H_2O] \text{ aprēķina dalot piesātinātu šķīdības produktu ar ūdeni } [H_2O].$$

$$\text{Piesātināti izšķīst } 94 \text{ g/L } SO_2 \text{ M} = 64,066 \text{ g/mol } [SO_2] = [H_2SO_3] = 94/64,066 = 1,46724 \text{ M sērskābes ar blīvumu}$$

$$1,05 \text{ g/mL } m_{\text{solution}} = 1050 \text{ g/L } M_{H_2SO_3} = 82,075 \text{ g/mol. Masu ūdenim dod } m_{H_2O} = 1050 - 120,4327 = 929,5673 \text{ g}$$

$$\text{skābes masa } m_{H_2SO_3} = [SO_2] \cdot M_{H_2SO_3} = 1,46724 \text{ M} \cdot 82,075 \text{ g/mol} = 120,4327 \text{ g/L. Ūdens koncentrācija konstantē ir}$$

$$n_{H_2O} = 929,5673/18 = 51,64 \text{ M. } SO_2^{gas} + H_2O = H_2SO_{3aq} \quad K_{eq} = [H_2SO_3]/[SO_2^{gas}]/[H_2O] = 1,46724/1/51,64 = 0,028413$$

$$\text{konstante dod } \Delta G_{eqH_2SO_3} = -R \cdot T \cdot \ln(K_{eq}) = -8,3144 \cdot 298,15 \cdot \ln(0,028413) = G_{H_2SO_3} - (G_{SO_2} + G_{H_2O}) = 8,82727 \text{ kJ/mol}$$

$$\text{brīvās enerģijas izmaiņu } \Delta G_{eqH_2SO_3} = G_{H_2SO_3} - (G_{SO_2} + G_{H_2O}) = 16,2761 - (7,44883 + 0) = 8,82727 \text{ kJ/mol}.$$

$$G_{SO_2}^{gas} = G_{H_2SO_3} - (\Delta G_{eqH_2SO_3} + G_{H_2O}) = 16,2761 - (8,82727 + 0) = 7,44883 \text{ kJ/mol}; 2 = -\text{pH} < 7 [17]$$

Veidošanās no brīvajiem elementiem $S_{\text{rombic}} + O_2^{\text{gas}} = SO_2^{\text{gas}}$: $\Delta G^{\circ}_{SO_2\text{Form}} = G_{SO_2} - (3,5436 + 303) = -300,1 \text{ kJ/mol}$;

$$G_{SO_2}^{\text{gas}} = \Delta G^{\circ}_{SO_2\text{Form}} + (G_{S_{\text{rombic}}} + G_{O_2}) = -300,1 + (3,5436 + 303,1) = 6,5436 \text{ kJ/mol};$$

Veidošanās no brīvajiem elementiem $S_{\text{rombic}} + 1,5O_2^{\text{gas}} + H_2^{\text{gas}} = H_2SO_3^{\text{aq}}$ un šķīdība $SO_2^{\text{gas}} + H_2O = H_2SO_3^{\text{aq}}$.

Viela	$\Delta H^{\circ}_{H_2O} \text{ kJ/mol}$	$\Delta S^{\circ}_{H_2O} \text{ J/mol/K}$	$\Delta G^{\circ}_{H_2O} \text{ kJ/mol}$
H₂O	-285,85	69,9565	-237,191
H₂O	-286,65	-453,188	-151,549
SO₃	-441,0	113,8	-373,8
SO₃	formation liq uid	-373,8	84,3936
H ₂ SO ₄	-814,0	156,9	-690,0
H ₂ SO ₄	formation liquid	-690	5,3436
H ₂ SO ₄	pK _{a1} =-2,8	protolysis	56,0585
HSO ₄ ⁻	-909,3	20,1	-744,5
HSO ₄ Ge-	formation	-744,5	119,54
HSO ₄ ⁻	pK _{a2} =1,99	protolysis	27,584
SO ₄ ²⁻ Ge-	formation	-744,5	80,603
SO ₄ ²⁻	-907,62	-536,2	-747,77
SO ₄ ²⁻ Ge-	formation[8]	-747,75	82,228
SO ₄ ²⁻	pK _{a2} =1,99	protolysis	26,4509
SO ₄ ²⁻	E° _{HSO₃} =	0,10726	26,44996
SO ₄ ²⁻	E° _{SO₃₂} =	0,05576	26,44996
SO ₄ ²⁻	E° _{SO₃₂} =	-1,2522	54,9256
SO ₂ ^{gas}	-296,81	248,223	-300,1
SO ₂ ^{gas}	formation	-300,1	6,5436
SO ₂ ^{gas}	K _{sp} =0,02841	2<pH<7	7,44883
H ₂ SO ₃	formation [8]	-509,736	34,0575
H ₂ SO ₃	pK _{a1} =1,857		34,0575
HSO ₃ ⁻	-626,2	139,7	-527,7
HSO ₃ ⁻	Ge- formation	-527,7	128,2536
HSO ₃ ⁻	pK _{a2} =7,172		32,125
HSO ₃ ⁻	E° _{HSO₃} =	0,10726	73,072
SO ₃ ²⁻	E° _{SO₃₂} =	0,05576	60,56996
SO ₃ ²⁻	-635,5	-29	-486,5
SO ₃ ²⁻	Ge-formation	-486,5	38,242
SO ₃ ²⁻	pK _{a2} =7,172		43,0036
SO ₃ ²⁻	E° _{SO₃₂-OH} =	-1,25223	141,8484

Biokīmijas ūdenim ir standarta brīvā enerģija $G_{H_2O} = 85,6 \text{ kJ/mol}$. [8]

$$G_{H_2O} = \Delta G_{H_2O} \text{Alberty} - (\Delta G^{\circ}_{H_2O}) = -151,549 - (-237,191) = 85,6 \text{ kJ/mol}.$$

$$\Delta G_H = \Delta H_H - T \cdot \Delta S_H = -286,65 - 298,15 \cdot (-0,453188) = -151,549 \text{ kJ/mol};$$

$$[1] \Delta G_H = \Delta H_H - T \cdot \Delta S_H = -441 - 298,15 \cdot 0,1138 = -474,92947 \text{ kJ/mol};$$

$$G_{SO_3} = \Delta G^{\circ}_{SO_3\text{Form}} + (G_{S_{\text{rombic}}} + 1,5G_{O_2}) = 84,3936 \text{ kJ/mol};$$

$$[1] \Delta G_H = \Delta H_H - T \cdot \Delta S_H = -814,0 - 298,15 \cdot 0,1569 = -860,78 \text{ kJ/mol};$$

$$G_{H_2SO_4} = \Delta G^{\circ}_{H_2SO_4} + G_{S_{\text{rombic}}} + 2\Delta G_{O_2} + G_{H_2}^{\text{gas}} + G_{H_2O} = 5,3436 \text{ kJ/mol};$$

$$G_{H_2SO_4} = G_{HSO_4} + G_{H_3O} - (\Delta G_{eqH_2SO_4} + G_{H_2O}) = 56,0585 \text{ kJ/mol};$$

$$[1] \Delta G = \Delta H - T \cdot \Delta S = -909,3 - 298,15 \cdot 0,0201 = -915,293 \text{ kJ/mol};$$

$$G_{Ge-} = G_{HSO_4} - (G_{S_{\text{rombic}}} + 2G_{O_2} + 0,5G_{H_2}^{\text{gas}} + \Delta G^{\circ}_{HSO_4}) = 119,54 \text{ kJ/mol};$$

$$G_{HSO_4} = \Delta G_{eqH_2SO_4} - G_{H_3O} + (G_{H_2SO_4} + G_{H_2O}) = 27,584 \text{ kJ/mol};$$

$$[1] 2G_{Ge-} = G_{SO_4^{2-}} - (G_{S_{\text{rombic}}} + 2G_{O_2} + \Delta G^{\circ}_{SO_4^{2-}}) = 161,2062 = 2 \cdot 80,60 \text{ kJ/mol};$$

$$[8] \Delta G_{SO_4^{2-}} = \Delta H - T \cdot \Delta S = -907,62 - 298,15 \cdot (-0,5362) = -747,75 \text{ kJ/mol};$$

$$[8] 2G_{Ge-} = G_{SO_4^{2-}} - (G_{S_{\text{rombic}}} + 2G_{O_2} + \Delta G^{\circ}_{SO_4^{2-}}) = 164,456 = 2 \cdot 82,228 \text{ kJ/mol};$$

$$G_{SO_4^{2-}} = \Delta G_{eqHSO_4} - G_{H_3O} + (G_{HSO_4} + G_{H_2O}) = 26,4509 \text{ kJ/mol}; 2 < \text{pH} < 7$$

$$G_{SO_4^{2-}} = \Delta G_{eqHSO_4^{2-}} - 3G_{H_3O} + (G_{HSO_3} + 4G_{H_2O}) = 26,44996 \text{ kJ/mol};$$

$$G_{SO_4^{2-}} = \Delta G_{eqSO_3^{2-}} - 2G_{H_3O} + (G_{SO_3^{2-}} + 3G_{H_2O}) = 26,44996 \text{ kJ/mol};$$

$$G_{SO_4^{2-}} = \Delta G_{eqSO_3^{2-}-OH} - G_{H_2O} + (G_{SO_3^{2-}} + 2G_{OH}) = 54,9256 \text{ kJ/mol};$$

$$[1] \Delta G_H = \Delta H_H - T \cdot \Delta S_H = -296,81 - 298,15 \cdot 0,248223 = -370,82 \text{ kJ/mol};$$

$$G_{SO_2} = \Delta G^{\circ}_{SO_2\text{Form}} + (G_{S_{\text{rombic}}} + G_{O_2}) = 6,5436 \text{ kJ/mol};$$

$$G_{SO_2}^{\text{gas}} = G_{H_2SO_3} - (\Delta G_{eqH_2SO_3} + G_{H_2O}) = 7,44883 \text{ kJ/mol};$$

$$G_{H_2SO_3} = \Delta G^{\circ}_{H_2SO_3} + (G_{S_{\text{rombic}}} + 1,5DG_{O_2} + G_{H_2}^{\text{gas}}) = 34,0575 \text{ kJ/mol};$$

$$G_{H_2SO_3} = G_{HSO_3} + G_{H_3O} - (\Delta G_{eqH_2SO_3} + G_{H_2O}) = 34,0575 \text{ kJ/mol}; \text{pH}=1,85$$

$$[1] \Delta G_H = \Delta H_H - T \cdot \Delta S_H = -626,2 - 298,15 \cdot 0,1397 = -667,85 \text{ kJ/mol};$$

$$G_{Ge-} = G_{HSO_3} - (G_{S_{\text{rombic}}} + 1,5\Delta G_{O_2} + G_{H_2}^{\text{gas}}/2 + \Delta G^{\circ}_{HSO_3}) = 128,2536 \text{ kJ/mol};$$

$$G_{HSO_3} = G_{SO_3^{2-}} + G_{H_3O} - (\Delta G_{eqHSO_3} + G_{H_2O}) = 32,125 \text{ kJ/mol};$$

$$G_{HSO_3} = G_{SO_4^{2-}} + 3G_{H_3O} - (\Delta G_{eqHSO_4} + 4G_{H_2O}) = 73,072 \text{ kJ/mol};$$

$$G_{SO_3^{2-}} = G_{SO_4^{2-}} - 2G_{H_3O} - (\Delta G_{eqSO_3^{2-}} + 3G_{H_2O}) = 60,56996 \text{ kJ/mol};$$

$$[1] \Delta G_H = \Delta H_H - T \cdot \Delta S_H = -635,5 - 298,15 \cdot (-0,029) = -626,85 \text{ kJ/mol};$$

$$2G_{Ge-} = G_{SO_3^{2-}} - (G_{S_{\text{rombic}}} + 1,5\Delta G_{O_2} + G_{H_2}^{\text{gas}}/2 + \Delta G^{\circ}_{SO_3^{2-}}) = 76,484 = 2 \cdot 38,24 \text{ kJ/mol};$$

$$G_{SO_3^{2-}} = \Delta G_{eqHSO_3} + G_{H_3O} - (G_{HSO_3} + G_{H_2O}) = 43,0036 \text{ kJ/mol}; \text{pH}=7,172;$$

$$G_{SO_3^{2-}} = G_{SO_4^{2-}} + G_{H_2O} - (\Delta G_{eqSO_3^{2-}-OH} + 2G_{OH}) = 141,8484 \text{ kJ/mol}; \text{pH}>7$$

https://en.wikipedia.org/wiki/Sulfurous_acid

[1] Protolīzes līdzsvaru molu daļās $K_{eq} = K_a/[H_2O]$ aprēķina dalot skābes konstanti ar ūdeni $[H_2O] = 55,3 \text{ M}$.

$$H_2SO_3 + H_2O = HSO_3^- + H_3O^+; pK_{a1} = 1,857; K_{eq1} = K_{a1}/[H_2O] = 10^{-(1,857)}/55,3 = 10^{-(3,5997251)} \text{ ir}$$

$$\Delta G_{eqH_2SO_3} = -R \cdot T \cdot \ln(K_{eq1}) = -8,3144 \cdot 298,15 \cdot \ln(10^{-(3,5997251)}) = 20,5075 \text{ kJ/mol}.$$

$$\Delta G_{eqH_2SO_3} = G_{HSO_3} + G_{H_3O} - (G_{H_2SO_3} + G_{H_2O}) = 32,125 + 22,44 - (34,0575 + 0) = 20,5075 \text{ kJ/mol}.$$

$$G_{H_2SO_3} = G_{HSO_3} + G_{H_3O} - (\Delta G_{eqH_2SO_3} + G_{H_2O}) = 32,125 + 22,44 - (20,5075 + 0) = 34,0575 \text{ kJ/mol}; \text{pH}=1,857$$

$$\text{Veidošana [8]} \Delta G^{\circ}_{H_2SO_3} = G_{H_2SO_3} - (G_{S_{\text{rombic}}} + 1,5DG_{O_2} + G_{H_2}^{\text{gas}}) = 34,0575 - (3,5436 + 1,5 \cdot 303,1 + 85,6) = -509,736 \text{ kJ/mol};$$

$$G_{H_2SO_3} = \Delta G^{\circ}_{H_2SO_3} + (G_{S_{\text{rombic}}} + 1,5DG_{O_2} + G_{H_2}^{\text{gas}}) = -509,736 + (3,5436 + 1,5 \cdot 303,1 + 85,6) = 34,0576 \text{ kJ/mol};$$

$$[1] \text{ protolīze } HSO_3^- + H_2O = SO_3^{2-} + H_3O^+; pK_{a2} = 7,172; K_{eq2} = K_{a2}/[H_2O] = 10^{-(7,172)}/55,3 = 10^{-(8,9147)};$$

$$\Delta G_{eqHSO_3} = -R \cdot T \cdot \ln(K_{eq2}) = -8,3144 \cdot 298,15 \cdot \ln(10^{-(8,9147)}) = 50,8848 \text{ kJ/mol};$$

$$\Delta G_{eqHSO_3} = G_{SO_3^{2-}} + G_{H_3O} - (G_{HSO_3} + G_{H_2O}) = 60,56996 + 22,44 - (32,125 + 0) = 50,8848 \text{ kJ/mol};$$

$$G_{SO_3^{2-}} = \Delta G_{eqHSO_3} + G_{H_3O} - (G_{HSO_3} + G_{H_2O}) = 50,8848 - 22,44 + (32,125 + 0) = 60,56996 \text{ kJ/mol};$$

$$G_{HSO_3} = G_{SO_3^{2-}} + G_{H_3O} - (\Delta G_{eqHSO_3} + G_{H_2O}) = 60,56996 + 22,44 - (50,8848 + 0) = 32,125 \text{ kJ/mol};$$

$$\text{Veidošana } HSO_3^- = S_{\text{rombic}} + 1,5O_2 + H_2^{\text{gas}}/2 + e^-; [1] SO_4^{2-} = S_{\text{rombic}} + 1,5O_2 + H_2^{\text{gas}}/2 + 2e^-; [1,8]$$

$$\text{Veidošana } \Delta G^{\circ}_{HSO_3} = G_{HSO_3} - (G_{S_{\text{rombic}}} + 1,5\Delta G_{O_2} + G_{H_2}^{\text{gas}}/2 + G_{e-}) = 101,54764 - (3,544 + 1,5 \cdot 303,1 + 85,6/2 + G_{e-}) = -527,7 \text{ kJ/mol};$$

$$G_{e-} = G_{HSO_3} - (G_{S_{\text{rombic}}} + 1,5\Delta G_{O_2} + G_{H_2}^{\text{gas}}/2 + \Delta G^{\circ}_{HSO_3}) = 101,54764 - (3,544 + 1,5 \cdot 303,1 + 85,6/2 - 527,7) = 128,2536 \text{ kJ/mol};$$

$$\text{Veidošana } \Delta G^{\circ}_{SO_3^{2-}} = G_{SO_3^{2-}} - (G_{S_{\text{rombic}}} + 1,5\Delta G_{O_2} + G_{H_2}^{\text{gas}}/2 + 2G_{e-}) = 90,9781 - (3,544 + 1,5 \cdot 303,1 + 85,6/2 + 2G_{e-}) = -486,5 \text{ kJ/mol};$$

$$2G_{e-} = G_{SO_3^{2-}} - (G_{S_{\text{rombic}}} + 1,5\Delta G_{O_2} + G_{H_2}^{\text{gas}}/2 + \Delta G^{\circ}_{SO_3^{2-}}) = 90,9781 - (3,544 + 1,5 \cdot 303,1 + 85,6/2 - 486,5) = 76,484 = 2 \cdot 38,242 \text{ kJ/mol};$$

2<pH<7 $HSO_3^- + 4H_2O = SO_4^{2-} + 3H_3O^+ + 2e^-$; Classic standarta potenciāls $E^{\circ}_{\text{classic}} = 0,172 \text{ V}$ [1], plus ūdens uzskaitē $-0,0591/2 \cdot \log(1/[H_2O]^4) = 0,206$ un saistītā summa $\Delta E^{\circ} = +0,10166 - 0,37239$ absolūtais potenciāls ir

$$E^{\circ}_{\text{HSO}_3^-} = E^{\circ} - 0,0591/2 \cdot \log(1/[\text{H}_2\text{O}]^4) + \Delta E^{\circ} = 0,172 - 0,0591/2 \cdot \log(1/55,3^4) + 0,10166 - 0,37239 = \mathbf{0,10726 \text{ V}};$$

$$2 < \text{pH} < 7 \quad E_{\text{HSO}_3^-} = E^{\circ}_{\text{HSO}_3^-} + 0,0591/2 \cdot \log \frac{[\text{SO}_4^{2-}] \cdot [\text{H}_3\text{O}^+]^3}{[\text{HSO}_3^-] \cdot [\text{H}_2\text{O}]^4} = \mathbf{0,10726 \text{ V}} + 0,0591/2 \cdot \log \frac{[\text{SO}_4^{2-}] \cdot [\text{H}_3\text{O}^+]^3}{[\text{HSO}_3^-] \cdot [\text{H}_2\text{O}]^4}$$

$$\Delta G_{\text{eqHSO}_3^-} = E^{\circ}_{\text{HSO}_4^-} \cdot F \cdot n = \mathbf{0,10726 \cdot 96485 \cdot 2 = 20,69796 \text{ kJ/mol}},$$

$$\Delta G_{\text{eqHSO}_3^-} = G_{\text{SO}_4^{2-}} + 3G_{\text{H}_3\text{O}^+} + 2G_{\text{e}^-} - (G_{\text{HSO}_3^-} + 4G_{\text{H}_2\text{O}}) = \mathbf{26,44996 + 3 \cdot 22,44 + 2 \cdot 0 - (73,072 + 4 \cdot 0) = 20,69797 \text{ kJ/mol}};$$

$$G_{\text{HSO}_3^-} = G_{\text{SO}_4^{2-}} + 3G_{\text{H}_3\text{O}^+} + 2G_{\text{e}^-} - (\Delta G_{\text{eqHSO}_3^-} + 4G_{\text{H}_2\text{O}}) = \mathbf{26,44996 + 3 \cdot 22,44 + 2 \cdot 0 - (20,69796 + 4 \cdot 0) = 73,072 \text{ kJ/mol}};$$

$$G_{\text{SO}_4^{2-}} = \Delta G_{\text{eqHSO}_3^-} - 3G_{\text{H}_3\text{O}^+} - 2G_{\text{e}^-} + (G_{\text{HSO}_3^-} + 4G_{\text{H}_2\text{O}}) = \mathbf{20,69796 - 3 \cdot 22,44 - 2 \cdot 0 + (73,072 + 4 \cdot 0) = 26,44996 \text{ kJ/mol}};$$

$$2G_{\text{e}^-} = \Delta G_{\text{eqHSO}_3^-} - 3G_{\text{H}_3\text{O}^+} - G_{\text{SO}_4^{2-}} + (G_{\text{HSO}_3^-} + 4G_{\text{H}_2\text{O}}) = \mathbf{20,69796 - 3 \cdot 22,44 - 26,44996 + (73,072 + 4 \cdot 0) = 2 \cdot 0 \text{ kJ/mol}};$$



pH > 7,21 $\text{SO}_3^{2-} + 3\text{H}_2\text{O} = \text{SO}_4^{2-} + 2\text{H}_3\text{O}^+ + 2\text{e}^-$; Classic standarta potenciāls $E^{\circ}_{\text{classic}} = 0,172 \text{ V}$ [1], plus ūdens uzskaitē $-0,0591/2 \cdot \log(1/[\text{H}_2\text{O}]^3) = 0,15449$ un saistītā summa $\Delta E^{\circ} = +0,10166 - 0,37239$ absolūtais potenciāls ir $E^{\circ}_{\text{H}_2\text{SO}_3} = E^{\circ}_{\text{Classic}} - 0,0591/2 \cdot \log(1/[\text{H}_2\text{O}]^3) + \Delta E^{\circ} = 0,172 - 0,0591/2 \cdot \log(1/55,3^3) + 0,10166 - 0,37239 = \mathbf{0,055763 \text{ V}};$

$$\text{pH} > 7,21 \quad E_{\text{HSO}_3^-} = E^{\circ}_{\text{HSO}_3^-} + 0,0591/2 \cdot \log \frac{[\text{SO}_4^{2-}] \cdot [\text{H}_3\text{O}^+]^2}{[\text{SO}_3^{2-}] \cdot [\text{H}_2\text{O}]^3} = \mathbf{0,055763 \text{ V}} + 0,0591/2 \cdot \log \frac{[\text{SO}_4^{2-}] \cdot [\text{H}_3\text{O}^+]^2}{[\text{SO}_3^{2-}] \cdot [\text{H}_2\text{O}]^3}$$

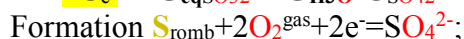
$$\Delta G_{\text{eqHSO}_3^-} = E^{\circ}_{\text{HSO}_3^-} \cdot F \cdot n = \mathbf{0,055763 \cdot 96485 \cdot 2 = 10,7600 \text{ kJ/mol}};$$

$$\Delta G_{\text{eqSO}_3^{2-}} = G_{\text{SO}_4^{2-}} + 2G_{\text{H}_3\text{O}^+} + 2G_{\text{e}^-} - (G_{\text{SO}_3^{2-}} + 3G_{\text{H}_2\text{O}}) = \mathbf{26,44996 + 2 \cdot 22,44 + 2 \cdot 0 - (60,56996 + 3 \cdot 0) = 10,7600 \text{ kJ/mol}};$$

$$G_{\text{SO}_4^{2-}} = \Delta G_{\text{eqSO}_3^{2-}} - 2G_{\text{H}_3\text{O}^+} - 2G_{\text{e}^-} + (G_{\text{SO}_3^{2-}} + 3G_{\text{H}_2\text{O}}) = \mathbf{10,7600 - 2 \cdot 22,44 - 2 \cdot 0 + (60,56996 + 3 \cdot 0) = 26,44996 \text{ kJ/mol}};$$

$$G_{\text{SO}_3^{2-}} = G_{\text{SO}_4^{2-}} + 2G_{\text{H}_3\text{O}^+} + 2G_{\text{e}^-} - (\Delta G_{\text{eqSO}_3^{2-}} + 3G_{\text{H}_2\text{O}}) = \mathbf{26,44996 + 2 \cdot 22,44 + 2 \cdot 0 - (10,7600 + 3 \cdot 0) = 60,56996 \text{ kJ/mol}};$$

$$2G_{\text{e}^-} = \Delta G_{\text{eqSO}_3^{2-}} - 2G_{\text{H}_3\text{O}^+} - G_{\text{SO}_4^{2-}} + (G_{\text{SO}_3^{2-}} + 3G_{\text{H}_2\text{O}}) = \mathbf{10,7600 - 2 \cdot 22,44 - 26,44996 + (60,56996 + 3 \cdot 0) = 2 \cdot 0 \text{ kJ/mol}};$$



$$\Delta G_{\text{SO}_4^{2-}} = G_{\text{SO}_4^{2-}} - (G_{\text{S}_{\text{romb}}} + G_{\text{O}_2^{\text{gas}}} + 2 \cdot G_{\text{e}^-}) = \mathbf{26,44996 - (3,5436 + 2 \cdot 303,1 + 2 \cdot 94,841) = -744,5 \text{ kJ/mol}};$$

$$2 \cdot G_{\text{e}^-} = G_{\text{SO}_4^{2-}} - (G_{\text{S}_{\text{romb}}} + 2 \cdot G_{\text{O}_2^{\text{gas}}} + \Delta G_{\text{SO}_4^{2-}}) = \mathbf{26,44996 - (3,5436 + 2 \cdot 303,1 - 744,5) = 161,20636 = 2 \cdot 80,60318 \text{ kJ/mol}};$$

$\text{SO}_3^{2-} + 2\text{OH}^- = \text{SO}_4^{2-} + \text{H}_2\text{O} + 2\text{e}^-$; pH > 7; Classic standarta potenciāls $E^{\circ}_{\text{Classic}} = -0,93 \text{ V}$ [17], ūdens uzskaitē $-0,0591/2 \cdot \log([\text{H}_2\text{O}]) = 0,0515$ un saistītā summa $\Delta E^{\circ} = +0,10166 - 0,37239$ izteiksmē absolūtais potenciāls ir $E^{\circ}_{\text{SO}_3^{2-}-\text{OH}} = E^{\circ}_{\text{Classic}} - 0,0591/2 \cdot \lg([\text{H}_2\text{O}]) + \Delta E^{\circ} = -0,93 - 0,0591/2 \cdot \log(55,3) + 0,10166 - 0,37239 = \mathbf{-1,25223 \text{ V}};$

$$E_{\text{SO}_3^{2-}-\text{OH}} = E^{\circ}_{\text{SO}_3^{2-}-\text{OH}} + \frac{0,0591}{2} \cdot \log \frac{[\text{SO}_4^{2-}] \cdot [\text{H}_2\text{O}]}{[\text{SO}_3^{2-}] \cdot [\text{OH}]^2} = \mathbf{-1,252 \text{ V}} + \frac{0,0591}{2} \cdot \log \frac{[\text{SO}_4^{2-}] \cdot [\text{H}_2\text{O}]}{[\text{SO}_3^{2-}] \cdot [\text{OH}]^2}$$

$$\Delta G_{\text{eqSO}_4^{2-}-\text{OH}} = E^{\circ}_{\text{SO}_3^{2-}-\text{OH}} \cdot F \cdot n = \mathbf{-1,25223 \cdot 96485 \cdot 2 = -241,6428 \text{ kJ/mol}};$$

$$\Delta G_{\text{eqSO}_3^{2-}-\text{OH}} = G_{\text{SO}_4^{2-}} + G_{\text{H}_2\text{O}} + 2G_{\text{e}^-} - (G_{\text{SO}_3^{2-}} + 2G_{\text{OH}^-}) = \mathbf{54,9256 + 0 + 2 \cdot 0 - (141,8484 + 2 \cdot 77,36) = -241,6428 \text{ kJ/mol}};$$

$$G_{\text{SO}_3^{2-}} = G_{\text{SO}_4^{2-}} + G_{\text{H}_2\text{O}} + 2G_{\text{e}^-} - (\Delta G_{\text{eqSO}_3^{2-}-\text{OH}} + 2G_{\text{OH}^-}) = \mathbf{54,9256 + 0 + 2 \cdot 0 - (-241,6428 + 2 \cdot 77,36) = 141,8484 \text{ kJ/mol}};$$

$$G_{\text{SO}_4^{2-}} = \Delta G_{\text{eqSO}_3^{2-}-\text{OH}} - G_{\text{H}_2\text{O}} - 2G_{\text{e}^-} + (G_{\text{SO}_3^{2-}} + 2G_{\text{OH}^-}) = \mathbf{-241,6428 - 0 - 2 \cdot 0 + (141,8484 + 2 \cdot 77,36) = 54,9256 \text{ kJ/mol}};$$

$$2G_{\text{e}^-} = \Delta G_{\text{eqSO}_3^{2-}-\text{OH}} - G_{\text{H}_2\text{O}} - G_{\text{SO}_4^{2-}} + (G_{\text{SO}_3^{2-}} + 2G_{\text{OH}^-}) = \mathbf{-241,6428 - 0 - 54,9256 + (141,8484 + 2 \cdot 77,36) = 2 \cdot 0 \text{ kJ/mol}};$$

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