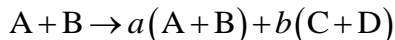
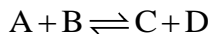


14-3-1 [BOY] For the reaction $A + B \leftrightarrow C + D$, Δg^{-o} is calculated to be 0 at 500 K.

Starting with a mixture of 1 kmol of A and 1 kmol of B, (a) evaluate what percent of the mixture is converted to products at equilibrium at 500 kPa, 500 K. (b) What would be the answer if the pressure (p) were 1000 kPa?

SOLUTION



$$y_{A+B} = \frac{a}{a+b+c+d}; \quad y_{C+D} = \frac{b}{a+b+c+d};$$

$$\begin{aligned} \text{(a)} \quad -\frac{\Delta \bar{g}_T^o}{RT} &= \ln K = \ln \left[\left(\frac{y_p^{v_p}}{y_r^{v_r}} \right) \left(\frac{p}{p_0} \right)^{\sum v_p - \sum v_r} \right]; \\ \Rightarrow -\frac{0}{R(500)} &= \ln \left[\left(\frac{y_{C+D}^{v_{C+D}}}{y_{A+B}^{v_{A+B}}} \right) \left(\frac{p}{p_0} \right)^{v_{C+D} - v_{A+B}} \right]; \quad \Rightarrow 0 = \ln \left[\left(\frac{y_{C+D}^1}{y_{A+B}^1} \right) \left(\frac{500}{p_0} \right)^{1-1} \right]; \\ \Rightarrow 0 &= \ln \left[\left(\frac{\left(\frac{b}{a+b+c+d} \right)}{\left(\frac{a}{a+b+c+d} \right)} \right) \left(\frac{500}{p_0} \right)^0 \right]; \quad \Rightarrow 1 = \left[\left(\frac{b}{a} \right) \right]; \quad \Rightarrow a = b; \end{aligned}$$

Therefore,

$$\begin{aligned} 1 &= a + b; \quad \Rightarrow 1 = a + a; \quad \Rightarrow 1 = 2a; \quad \Rightarrow a = 0.5; \\ \Rightarrow b &= 1 - a = 1 - 0.5 = 0.5 = \mathbf{50\%} \end{aligned}$$

$$\begin{aligned} \text{(b)} \quad -\frac{\Delta \bar{g}_T^o}{RT} &= \ln K = \ln \left[\left(\frac{y_p^{v_p}}{y_r^{v_r}} \right) \left(\frac{p}{p_0} \right)^{\sum v_p - \sum v_r} \right]; \\ \Rightarrow -\frac{0}{R(500)} &= \ln \left[\left(\frac{y_{C+D}^{v_{C+D}}}{y_{A+B}^{v_{A+B}}} \right) \left(\frac{p}{p_0} \right)^{v_{C+D} - v_{A+B}} \right]; \quad \Rightarrow 0 = \ln \left[\left(\frac{y_{C+D}^1}{y_{A+B}^1} \right) \left(\frac{1000}{p_0} \right)^{1-1} \right]; \\ \Rightarrow 0 &= \ln \left[\left(\frac{\left(\frac{b}{a+b+c+d} \right)}{\left(\frac{a}{a+b+c+d} \right)} \right) \left(\frac{1000}{p_0} \right)^0 \right]; \quad \Rightarrow 1 = \left[\left(\frac{b}{a} \right) \right]; \quad \Rightarrow a = b; \end{aligned}$$

Therefore,

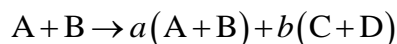
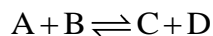
$$1 = a + b; \quad \Rightarrow 1 = a + a; \quad \Rightarrow 1 = 2a; \quad \Rightarrow a = 0.5;$$

$$\Rightarrow b = 1 - a = 1 - 0.5 = 0.5 = 50\%$$

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14-3-2 [BOF] For an elementary step $A + B \leftrightarrow C + D$, Δg^{-o} is tabulated as 22.819 at 298 K, 0 at 1000 K, and -229.724 MJ/kmol at 3000 K. Starting with a mixture of 1 kmol of A and 1 kmol of B, evaluate what percent of the mixture is converted to products at equilibrium at (a) 298 K, (b) 1000 K, and (c) 3000 K.

SOLUTION



$$y_{A+B} = \frac{a}{a+b+c+d}; \quad y_{C+D} = \frac{b}{a+b+c+d};$$

$$\begin{aligned} \text{(a)} \quad -\frac{\Delta \bar{g}_T^o}{RT} &= \ln K = \ln \left[\left(\frac{y_p^{v_p}}{y_r^{v_r}} \right) \left(\frac{p}{p_0} \right)^{\sum_p v_p - \sum_r v_r} \right]; \\ &\Rightarrow -\frac{22819}{(8.314)(298)} = \ln \left[\left(\frac{y_{C+D}^{v_{C+D}}}{y_{A+B}^{v_{A+B}}} \right) \left(\frac{p}{p_0} \right)^{v_{C+D} - v_{A+B}} \right]; \Rightarrow -9.210227 = \ln \left[\left(\frac{y_{C+D}^1}{y_{A+B}^1} \right) \left(\frac{1}{p_0} \right)^{1-1} \right]; \\ &\Rightarrow -9.210227 = \ln \left[\left(\frac{\left(\frac{b}{a+b+c+d} \right)}{\left(\frac{a}{a+b+c+d} \right)} \right) \left(\frac{1}{p_0} \right)^0 \right]; \Rightarrow 1.00011 \times 10^{-4} = \left[\frac{b}{a} \right]; \\ &\Rightarrow 1.00011 \times 10^{-4} a = b; \end{aligned}$$

Therefore,

$$\begin{aligned} 1 &= a + b; \quad \Rightarrow 1 = a + 1.00011 \times 10^{-4} a; \quad \Rightarrow 1 = 1.0001a; \quad \Rightarrow a = 0.99; \\ &\Rightarrow b = 1 - a = 1 - 0.99 = 0.01 = \mathbf{1\%} \end{aligned}$$

$$\text{(b)} \quad -\frac{\Delta \bar{g}_T^o}{RT} = \ln K = \ln \left[\left(\frac{y_p^{v_p}}{y_r^{v_r}} \right) \left(\frac{p}{p_0} \right)^{\sum_p v_p - \sum_r v_r} \right];$$

$$\Rightarrow -\frac{0}{(8.314)(1000)} = \ln \left[\left(\frac{y_{C+D}^{v_{C+D}}}{y_{A+B}^{v_{A+B}}} \right) \left(\frac{p}{p_o} \right)^{v_{C+D} - v_{A+B}} \right]; \quad \Rightarrow 0 = \ln \left[\left(\frac{y_{C+D}^1}{y_{A+B}^1} \right) \left(\frac{1}{p_o} \right)^{1-1} \right];$$

$$\Rightarrow 0 = \ln \left[\left(\frac{\left(\frac{b}{a+b+c+d} \right)}{\left(\frac{a}{a+b+c+d} \right)} \right) \left(\frac{1}{p_o} \right)^0 \right]; \quad \Rightarrow 1 = \left[\frac{b}{a} \right];$$

$$\Rightarrow a = b;$$

Therefore,

$$1 = a + b; \quad \Rightarrow 1 = a + a; \quad \Rightarrow 1 = 2a; \quad \Rightarrow a = 0.5;$$

$$\Rightarrow b = 1 - a = 1 - 0.5 = 0.5 = \text{50\%}$$

$$(c) \quad -\frac{\Delta \bar{g}_T^o}{RT} = \ln K = \ln \left[\left(\frac{y_p^{v_p}}{y_r^{v_r}} \right) \left(\frac{p}{p_o} \right)^{\sum_p v_p - \sum_r v_r} \right];$$

$$\Rightarrow -\frac{-229724}{(8.314)(3000)} = \ln \left[\left(\frac{y_{C+D}^{v_{C+D}}}{y_{A+B}^{v_{A+B}}} \right) \left(\frac{p}{p_o} \right)^{v_{C+D} - v_{A+B}} \right]; \quad \Rightarrow 9.210327961 = \ln \left[\left(\frac{y_{C+D}^1}{y_{A+B}^1} \right) \left(\frac{1}{p_o} \right)^{1-1} \right];$$

$$\Rightarrow 9.210327961 = \ln \left[\left(\frac{\left(\frac{b}{a+b+c+d} \right)}{\left(\frac{a}{a+b+c+d} \right)} \right) \left(\frac{1}{p_o} \right)^0 \right]; \quad \Rightarrow 9999.79 = \left[\frac{b}{a} \right];$$

$$\Rightarrow 9999.79a = b;$$

Therefore,

$$1 = a + b; \quad \Rightarrow 1 = a + 9999.79a; \quad \Rightarrow 1 = 10000.79a; \quad \Rightarrow a = 9.99 \times 10^{-5};$$

$$\Rightarrow b = 1 - a = 1 - (9.99 \times 10^{-5}) = 0.99 = \text{99\%}$$

14-3-3 [BOD] Evaluate Δg° at 298 K for the reaction $\text{H}_2 + (1/2)\text{O}_2 \leftrightarrow \text{H}_2\text{O}$ using (a) fundamental definition using formation enthalpy (h°_f) and entropy (s°) values, and (b) using formation Gibbs function from Table G-1.

SOLUTION



Given: $T = 298$;

$$(a) \quad \bar{g}_T^\circ = \Delta \left[\bar{h}(p_o, T) - T\bar{s}(p_o, T) \right] = \Delta \bar{h}(T) - T\Delta \bar{s}^\circ(T);$$

Handling the enthalpy term first and using Table G-1 we get,

$$\Delta \bar{h}(T) = \bar{h}_p(T) - \bar{h}_r(T) = \sum_p \nu_p \bar{h}_p(T) - \sum_r \nu_r \bar{h}_r(T);$$

$$\Rightarrow \Delta \bar{h}(T) = \nu_{\text{H}_2\text{O}} \bar{h}_{f, \text{H}_2\text{O}} - \nu_{\text{H}_2} \bar{h}_{f, \text{H}_2} - \nu_{\text{O}_2} \bar{h}_{f, \text{O}_2};$$

$$\Rightarrow \Delta \bar{h}(T) = (1)(-241,820) - (1)(0) - (0.5)(0);$$

$$\Rightarrow \Delta \bar{h}(T) = -241,820 \frac{\text{kJ}}{\text{kmol}}$$

And then evaluating entropy and using the Table G-1,

$$\Delta \bar{s}^\circ(T) = \sum_p \nu_p \bar{s}_p^\circ(T) - \sum_r \nu_r \bar{s}_r^\circ(T);$$

$$\Rightarrow \Delta \bar{s}^\circ(T) = \nu_{\text{H}_2\text{O}} \bar{s}_{\text{H}_2\text{O}}^\circ @ 298 \text{ K} - \nu_{\text{H}_2} \bar{s}_{\text{H}_2}^\circ @ 298 \text{ K} - \nu_{\text{O}_2} \bar{s}_{\text{O}_2}^\circ @ 298 \text{ K};$$

$$\Rightarrow \Delta \bar{s}^\circ(T) = (1)(188.83) - (1)(130.68) - (0.5)(205.04);$$

$$\Rightarrow \Delta \bar{s}^\circ(T) = -44.37 \frac{\text{kJ}}{\text{kmol} \cdot \text{K}}$$

Combining all the terms now we obtain,

$$\Delta \bar{g}_T^\circ = \Delta \bar{h}(T) - T\Delta \bar{s}^\circ(T);$$

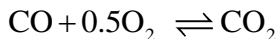
$$\Rightarrow \Delta \bar{g}_T^\circ = -241,820 - (298)(-44.37);$$

$$\Rightarrow \Delta \bar{g}_T^\circ = -228,597 \frac{\text{kJ}}{\text{kmol}}$$

(b) Now using Gibb's formation function from Table G.1 and realizing that we only need to look up one value for water vapor we find that $\bar{g}_f^\circ = -228,590 \frac{\text{kJ}}{\text{kmol}}$, which is very close to what we had before in part (a).

14-3-4 [BOM] Evaluate (a) Δh° , (b) Δg° , and (c) $\ln K$ at 298 K for the reaction $\text{CO} + 1/2\text{O}_2 \leftrightarrow \text{CO}_2$ at 1 atm.

SOLUTION



Given: $T = 298 \text{ K}$; $p_0 = 1 \text{ atm}$

(a) Handling the enthalpy term first and using Table G-1 we get,

$$\begin{aligned}\Delta \bar{h}(T) &= \bar{h}_p(T) - \bar{h}_r(T) = \sum_p \nu_p \bar{h}_p(T) - \sum_r \nu_r \bar{h}_r(T); \\ \Rightarrow \Delta \bar{h}^\circ &= \nu_{\text{CO}_2} \bar{h}_{f,\text{CO}_2} - \nu_{\text{CO}} \bar{h}_{f,\text{CO}} - \nu_{\text{O}_2} \bar{h}_{f,\text{O}_2}; \\ \Rightarrow \Delta \bar{h}^\circ &= (1)(-393,520) - (1)(-110,530) - (0.5)(0); \\ \Rightarrow \Delta \bar{h}^\circ &= -282990 \frac{\text{kJ}}{\text{kmol}} = -282.99 \frac{\text{MJ}}{\text{kmol}}\end{aligned}$$

(b) $\Delta \bar{g}_T^\circ = \Delta [\bar{h}(p_0, T) - T\bar{s}(p_0, T)] = \Delta \bar{h}(T) - T\Delta \bar{s}^\circ(T);$

And then evaluating entropy and using the IG tables:

$$\begin{aligned}\Delta \bar{s}^\circ(T) &= \sum_p \nu_p \bar{s}_p^\circ(T) - \sum_r \nu_r \bar{s}_r^\circ(T); \\ \Rightarrow \Delta \bar{s}^\circ &= \nu_{\text{CO}_2} \bar{s}_{\text{CO}_2@298\text{K}}^\circ - \nu_{\text{CO}} \bar{s}_{\text{CO}@298\text{K}}^\circ - \nu_{\text{O}_2} \bar{s}_{\text{O}_2@298\text{K}}^\circ; \\ \Rightarrow \Delta \bar{s}^\circ &= (1)(213.685) - (1)(197.543) - (0.5)(205.0); \\ \Rightarrow \Delta \bar{s}^\circ &= -86.358 \frac{\text{kJ}}{\text{kmol} \cdot \text{K}}\end{aligned}$$

Combining all the terms now we obtain,

$$\begin{aligned}\Delta \bar{g}_T^\circ &= \Delta \bar{h}(T) - T\Delta \bar{s}^\circ(T); \\ \Rightarrow \Delta \bar{g}_T^\circ &= -282990 - (298)(-86.358); \\ \Rightarrow \Delta \bar{g}_T^\circ &= -257,255 = -257.255 \frac{\text{MJ}}{\text{kmol}}\end{aligned}$$

(c) $\ln K = -\frac{\Delta \bar{g}_T^\circ}{RT};$

$$\begin{aligned}\Rightarrow \ln K &= -\frac{-257,255}{(8.314)(298)}; \\ \Rightarrow \ln K &= 103.83\end{aligned}$$

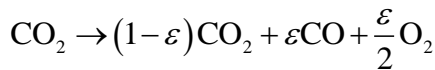
14-3-5 [BOW] A mixture of CO_2 , CO and O_2 is in equilibrium at a specified temperature and pressure. Now the pressure is tripled, (a) will the equilibrium constant K change? (b) Will the number of moles of CO_2 , CO and O_2 change? How? (Enter 1 if increases, 2 if decreases, and 3 if no change)

SOLUTION



$$\text{C balance: } 1 = (1-\varepsilon) + a; \quad \Rightarrow a = \varepsilon$$

$$\text{O balance: } 2 = 2(1-\varepsilon) + a + 2b; \quad \Rightarrow b = \frac{\varepsilon}{2}$$



Therefore,

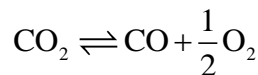
$$(1-\varepsilon) + a + b = 1 - \varepsilon + \varepsilon + \frac{\varepsilon}{2} = \frac{2+\varepsilon}{2}$$

$$y_{\text{CO}_2} = \frac{2(1-\varepsilon)}{2+\varepsilon}; \quad y_{\text{CO}} = \frac{2\varepsilon}{2+\varepsilon}; \quad y_{\text{O}_2} = \frac{\varepsilon}{2+\varepsilon}$$

From the equilibrium equation:

$$-\frac{\Delta \bar{g}_r^o}{RT} = \ln K = \ln \left[\left(\frac{\prod_p y_p^{v_p}}{\prod_r y_r^{v_r}} \right) \left(\frac{p}{p_0} \right)^{\sum_p v_p - \sum_r v_r} \right];$$

The associated elementary step,



$$K = \left[\left(\frac{y_{\text{CO}}^1 y_{\text{O}_2}^{0.5}}{y_{\text{CO}_2}^1} \right) \left(\frac{p}{p_0} \right)^{1.5-1} \right];$$

(a) If pressure is tripled and temperature and number of moles is held constant:

The equilibrium constant is independent of the pressure at a given temperature, any change in pressure is absorbed by a change in mole fraction.

Therefore, K remains the same: 3

(b) If pressure is tripled and temperature and K is held constant:

$$K_1 = \left[\left(\frac{\prod_p y_p^{v_p}}{\prod_r y_r^{v_r}} \right) \left(\frac{3p}{p_0} \right)^{\sum_p v_p - \sum_r v_r} \right] = (3)^{\sum_p v_p - \sum_r v_r} \left[\left(\frac{\prod_p y_p^{v_p}}{\prod_r y_r^{v_r}} \right) \left(\frac{p}{p_0} \right)^{\sum_p v_p - \sum_r v_r} \right]$$

Since we know K remains constant, the change in right hand side of the above equation due to the change in the $(p / p_0)^{\sum_p v_p - \sum_r v_r}$ term has to be canceled out. For the given reaction v_p and v_r are fixed quantities, and $\sum_p v_p - \sum_r v_r = 0.5$, which is positive, so any increase in p will result in a larger pressure term. Tripling the pressure results in $(3)^{0.5} (p / p_0)^{0.5}$. In order to nullify this, the product term must decrease in response, and since v_p and v_r are fixed, y_p and y_r are the only terms that can change. Therefore to keep the right hand side of the equation constant by cancelling out the $3^{0.5}$, the concentration of the reactant has to increase and the concentration of the product has to decrease. Therefore,

$\text{CO}_2 =$ increases: 1

$\text{CO} =$ decreases: 2

$\text{O}_2 =$ decreases: 2

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14-3-6 [BBR] Suppose the equilibrium constant of the dissociation reaction $\text{H}_2 \rightleftharpoons 2\text{H}$ at 2000 K and 1 atm is K_1 . Express the equilibrium constants of the following reactions at 2000 K in terms of K_1 : (a) $\text{H}_2 \rightleftharpoons 2\text{H}$ at 4 atm, (b) $2\text{H} \rightleftharpoons \text{H}_2$ at 1 atm, (c) $2\text{H}_2 \rightleftharpoons 4\text{H}$ at 1 atm, (d) $\text{H}_2 + 2\text{N}_2 \rightleftharpoons 2\text{H} + 2\text{N}_2$ at 2 atm and (e) $6\text{H} \rightleftharpoons 3\text{H}_2$ at 4 atm.

SOLUTION

Using the ideal gas model assumption, a specific equation for calculating the equilibrium constant will be used in finding the new equilibrium constant with respect to K_1 . The temperature of parts a through e do not change so no major calculations of enthalpy nor entropy need to be made.

The equation used is:

$$K = \left(\frac{y_p^{v_p}}{y_r^{v_r}} \right) \left(\frac{p}{p_0} \right)^{\sum v_p - \sum v_r}$$

Where $p_0 = 1 \text{ atm}$, $y_k = \text{mole fraction}$

$$y_i = \frac{n_i}{n_{\text{total}}}$$

The inverse reaction is the reciprocal of K , therefore:

$$K_{\text{inverse}} = \frac{1}{K}$$

In another form:

$$\log_{10} K_{\text{inverse}} = -\log_{10} K$$

For the case of K_1 :

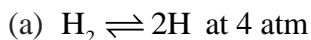
$$y_r = \frac{1}{3}$$

$$y_p = \frac{2}{3}$$

$$\ln K_1 = \ln \left[\left(\frac{0.66^2}{0.33^1} \right) \left(\frac{1 \text{ atm}}{1 \text{ atm}} \right)^{2-1} \right] = \ln \left[\frac{4}{3} \right]$$

$$K_1 = \frac{4}{3}$$

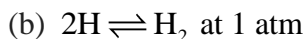
With these equations, part a through e can be solved.



$$K = \left[\left(\frac{0.66^2}{0.33^1} \right) \left(\frac{4 \text{ atm}}{1 \text{ atm}} \right)^{2-1} \right] = \frac{16}{3}$$

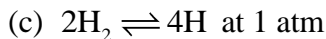
Therefore,

$$K = 4K_1$$



This is the inverse of the original reaction. Therefore,

$$K = \frac{1}{K_1}$$

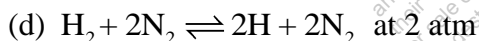


The mole fractions of the reactants and products are still the same even though there are more kmols of products and reactants. Since the pressure ratio is equal to one the equilibrium constant doesn't change. Therefore,

$$K = \left[\left(\frac{0.66^2}{0.33^1} \right) \left(\frac{1 \text{ atm}}{1 \text{ atm}} \right)^{4-2} \right] = \frac{4}{3}$$

Therefore,

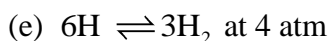
$$K = K_1$$



$$K = \left[\left(\frac{\left(\frac{2}{7} \right)^2 \left(\frac{2}{7} \right)^2}{\left(\frac{1}{7} \right)^1 \left(\frac{2}{7} \right)^2} \right) \left(\frac{2 \text{ atm}}{1 \text{ atm}} \right)^{4-3} \right] = \frac{24}{21}$$

Therefore,

$$K = \frac{6}{7} K_1$$



$$K = \left[\frac{\left(\frac{3}{9}\right)^3}{\left(\frac{6}{9}\right)^6} \left(\frac{4 \text{ atm}}{1 \text{ atm}}\right)^{3-6} \right] = 0.0049 \left[\frac{4}{3} \right]$$

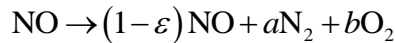
Therefore,

$$K = 0.0049 K_1$$

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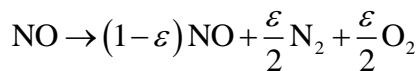
14-3-7 [BBB] A mixture of NO, O₂ and N₂ is in equilibrium at a specified temperature and pressure. The pressure is doubled, (a) will the equilibrium constant K change? (b) Will the number of moles of NO, O₂ and N₂, change? How?

SOLUTION



$$\text{N balance: } 1 = (1-\varepsilon) + 2a; \quad \Rightarrow a = \frac{\varepsilon}{2}$$

$$\text{O balance: } 1 = (1-\varepsilon) + 2b; \quad \Rightarrow b = \frac{\varepsilon}{2}$$



Therefore

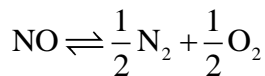
$$(1-\varepsilon) + a + b = 1 - \varepsilon + \frac{\varepsilon}{2} + \frac{\varepsilon}{2} = 1$$

$$y_{\text{NO}} = 1-\varepsilon; \quad y_{\text{N}_2} = \frac{\varepsilon}{2}; \quad y_{\text{O}_2} = \frac{\varepsilon}{2}$$

From the equilibrium equation:

$$-\frac{\Delta \bar{g}_T^o}{RT} = \ln K = \ln \left[\left(\frac{\prod_p y_p^{v_p}}{\prod_r y_r^{v_r}} \right) \left(\frac{p}{p_o} \right)^{\sum v_p - \sum v_r} \right];$$

The associated elementary step,



$$K = \left[\left(\frac{y_{\text{N}_2}^{0.5} y_{\text{O}_2}^{0.5}}{y_{\text{NO}}^1} \right) \left(\frac{p}{p_0} \right)^{1-1} \right]$$

(a) If pressure is doubled and temperature and number of moles is held constant:

The equilibrium constant is independent of the pressure at a given temperature, any change in pressure is absorbed by a change in mole fraction.

Therefore, K **remains the same: 3**

(b) If pressure is doubled and temperature and K is held constant:

$$K_1 = \left[\left(\frac{\prod_p y_p^{v_p}}{\prod_r y_r^{v_r}} \right) \left(\frac{2p}{p_0} \right)^{\sum_p v_p - \sum_r v_r} \right] = (2)^{\sum_p v_p - \sum_r v_r} \left[\left(\frac{\prod_p y_p^{v_p}}{\prod_r y_r^{v_r}} \right) \left(\frac{p}{p_0} \right)^{\sum_p v_p - \sum_r v_r} \right]$$

We know that K is a constant, so the $(2)^{\sum_p v_p - \sum_r v_r}$ has to be canceled out. We know that for this reaction v_p and v_r are fixed, and as such for this case $\sum_p v_p - \sum_r v_r = 0$, so

$(2)^{\sum_p v_p - \sum_r v_r} = 1$ and the change in pressure has no effect on the right hand side of the equation. Therefore the concentrations will not change.

NO = **no change: 3**

N₂ = **no change: 3**

O₂ = **no change: 3**

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14-3-8 [BOJ] Suppose the equilibrium constant of the reaction $\text{CO} + 1/2\text{O}_2 \rightleftharpoons \text{CO}_2$ at 1500 K and 1 atm is K_1 . Express the equilibrium constant of the following reactions at 1500 K in terms of K_1 . (a) $\text{CO} + (1/2)\text{O}_2 \rightleftharpoons \text{CO}_2$ at 2 atm, (b) $\text{CO}_2 \rightleftharpoons \text{CO} + (1/2)\text{O}_2$ at 1 atm, (c) $\text{CO} + \text{O}_2 \rightleftharpoons \text{CO}_2 + (1/2)\text{O}_2$ at 1 atm, (d) $\text{CO} + 2\text{O}_2 + 6\text{N}_2 \rightleftharpoons \text{CO}_2 + 1.5\text{O}_2 + 6\text{N}_2$ at 5 atm and (e) $2\text{CO} + \text{O}_2 \rightleftharpoons 2\text{CO}_2$.

SOLUTION

Using the ideal gas model assumption, a specific equation for calculating the equilibrium constant will be used in finding the new equilibrium constant with respect to K_1 . The temperature of parts a through e do not change so no major calculations of enthalpy or entropy need to be made.

The equation used is:

$$K = \left(\frac{y_p^{v_p}}{y_r^{v_r}} \right) \left(\frac{p}{p_0} \right)^{\sum v_p - \sum v_r}$$

Where $p_0 = 1 \text{ atm}$, $y_k = \text{mole fraction}$

$$y_i = \frac{n_i}{n_{\text{total}}};$$

The inverse reaction is the reciprocal of K , therefore:

$$K_{\text{inverse}} = \frac{1}{K}$$

In another form:

$$\log_{10} K_{\text{inverse}} = -\log_{10} K$$

For the case of K_1 :

$$\ln K_1 = \ln \left[\frac{\left(\frac{1}{2.5} \right)^1}{\left(\frac{1}{2.5} \right)^1 \left(\frac{0.5}{2.5} \right)^{0.5}} \left(\frac{1 \text{ atm}}{1 \text{ atm}} \right)^{1-1.5} \right] = \ln [2.236]$$

$$K_1 = 2.236$$

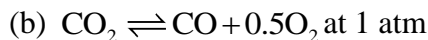
With these equations, part a through e can be solved.

(a) $\text{CO} + 0.5\text{O}_2 \rightleftharpoons \text{CO}_2$ at 2 atm

$$K = \left[\frac{\left(\frac{1}{2.5} \right)^1}{\left(\frac{1}{2.5} \right)^1 \left(\frac{0.5}{2.5} \right)^{0.5}} \left(\frac{2 \text{ atm}}{1 \text{ atm}} \right)^{1-1.5} \right] = 3.549$$

Therefore,

$$K = 2^{-0.5} K_1$$



This is the inverse of the original reaction. Therefore,

$$K = \frac{1}{K_1}$$



$$K = \left[\frac{\left(\frac{1}{3.5} \right)^1 \left(\frac{0.5}{3.5} \right)^{0.5}}{\left(\frac{1}{3.5} \right)^1 \left(\frac{1}{3.5} \right)^1} \left(\frac{1 \text{ atm}}{1 \text{ atm}} \right)^{1.5-2} \right] = 1.3229$$

Therefore,

$$K = 0.5916 K_1$$



$$K = \left[\frac{\left(\frac{1}{17.5} \right)^1 \left(\frac{1.5}{17.5} \right)^{1.5} \left(\frac{6}{17.5} \right)^6}{\left(\frac{1}{17.5} \right)^1 \left(\frac{2}{17.5} \right)^2 \left(\frac{6}{17.5} \right)^6} \left(\frac{5 \text{ atm}}{1 \text{ atm}} \right)^{8.5-9} \right] = 0.8592$$

Therefore,

$$K = 0.3843 K_1$$



$$K = \left[\frac{\left(\frac{2}{5} \right)^2}{\left(\frac{2}{5} \right)^2 \left(\frac{1}{5} \right)^1} \left(\frac{1 \text{ atm}}{1 \text{ atm}} \right)^{2-3} \right] = 5$$

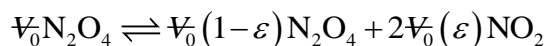
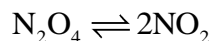
Therefore,

$$K = K_1^2$$

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14-3-9 [BBO] For the dissociation of nitrogen tetroxide according to the reaction, $\text{N}_2\text{O}_4 \rightleftharpoons 2\text{NO}_2$, show that the degree of dissociation at equilibrium is given by $\varepsilon = V_e/V_0 - 1$, where V_0 is the initial volume and V_e is the equilibrium volume.

SOLUTION



Therefore,

$$V_e = V_0 - V_0\varepsilon + 2V_0\varepsilon = V_0 + V_0\varepsilon;$$

$$\Rightarrow V_e = V_0(1 + \varepsilon);$$

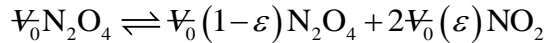
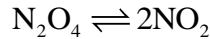
$$\Rightarrow \frac{V_e}{V_0} = (1 + \varepsilon);$$

$$\Rightarrow \varepsilon = \frac{V_e}{V_0} - 1$$

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14-3-10 [BBH] For the dissociation of nitrogen tetroxide described in problem 14-3-9 [BBO], there is a 77.7% increase in volume when equilibrium is reached at 50°C, 125 kPa. Determine the value of the equilibrium constant (K).

SOLUTION



Therefore,

$$V_e = V_0 - V_0\varepsilon + 2V_0\varepsilon = V_0 + V_0\varepsilon;$$

$$\Rightarrow V_e = V_0(1 + \varepsilon);$$

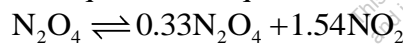
$$\Rightarrow \frac{V_e}{V_0} = (1 + \varepsilon);$$

$$\Rightarrow \varepsilon = \frac{V_e}{V_0} - 1$$

For this problem, we will assume that the initial volume is 1 m³, making the equilibrium volume equal to 1.77 m³. Solving for the dissociation,

$$\varepsilon = \frac{V_e}{V_0} - 1 = \frac{1.77}{1} - 1 = 0.77$$

The equilibrium equation now becomes:



$$y_{\text{N}_2\text{O}_4} = \frac{0.33}{1.87}; \quad y_{\text{NO}_2} = \frac{1.54}{1.87}$$

$$\ln K = \ln \left[\left(\frac{y_p^{v_p}}{y_r^{v_r}} \right) \left(\frac{P}{P_0} \right)^{\sum_p v_p - \sum_r v_r} \right] = \ln \left[\left(\frac{y_{\text{NO}_2}^{v_{\text{NO}_2}}}{y_{\text{N}_2\text{O}_4}^{v_{\text{N}_2\text{O}_4}}} \right) \left(\frac{P}{P_0} \right)^{v_{\text{NO}_2} - v_{\text{N}_2\text{O}_4}} \right] = \ln \left[\frac{\left(\frac{1.54}{1.87} \right)^2}{\left(\frac{0.33}{1.87} \right)} \left(\frac{125}{100} \right)^{2-1} \right];$$

$$\Rightarrow \ln K = \ln(4.81);$$

$$\Rightarrow K = 4.81$$

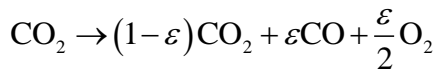
14-3-11 [BBS] A chamber contains a mixture of CO₂, CO and O₂ is in equilibrium at a specified temperature and pressure. How will (a) increasing the temperature (T) at constant pressure and (b) increasing the pressure (p) at constant temperature affect the number of moles of CO? (Enter 1 if increases, 2 if decreases, and 3 if no change)

SOLUTION



$$\text{C balance: } 1 = (1-\varepsilon) + a; \quad \Rightarrow a = \varepsilon$$

$$\text{O balance: } 2 = 2(1-\varepsilon) + a + 2b; \quad \Rightarrow b = \frac{\varepsilon}{2}$$



Therefore,

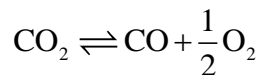
$$(1-\varepsilon) + a + b = 1 - \varepsilon + \varepsilon + \frac{\varepsilon}{2} = \frac{2+\varepsilon}{2}$$

$$y_{\text{CO}_2} = \frac{2(1-\varepsilon)}{2+\varepsilon}; \quad y_{\text{CO}} = \frac{2\varepsilon}{2+\varepsilon}; \quad y_{\text{O}_2} = \frac{\varepsilon}{2+\varepsilon}$$

From the equilibrium equation:

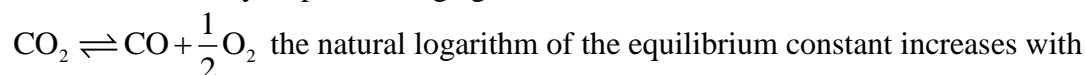
$$-\frac{\Delta \bar{g}_T^o}{RT} = \ln K = \ln \left[\left(\frac{\prod_p y_p^{v_p}}{\prod_r y_r^{v_r}} \right) \left(\frac{p}{p_o} \right)^{\sum_p v_p - \sum_r v_r} \right];$$

The associated elementary step,



$$K = \left[\left(\frac{y_{\text{CO}}^1 y_{\text{O}_2}^{0.5}}{y_{\text{CO}_2}^1} \right) \left(\frac{p}{p_0} \right)^{1.5-1} \right];$$

(a) For this elementary step, checking against Table G-3, we can see that for



temperature. As such, the concentration of the products must increase (and the reactants decrease) to match this change since there is no pressure effect. Therefore, the moles of CO must **increase: 1**

(b) Again, looking at the above expression, it can be seen that when the temperature is at a constant specified value, in order to keep the value $\ln K$ the same, the number of moles of products must decrease to offset the effect of the pressure increase since

$\sum_p v_p - \sum_r v_r = 0.5$. This causes the number of moles of CO to **decrease: 2**

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14-3-12 [BBA] Determine the change in the Gibbs function $\Delta g^{-\circ}$ at 25°C , in kJ/kmol , for the reaction $\text{CH}_4(\text{g}) + 2\text{O}_2 \leftrightarrow \text{CO}_2 + 2\text{H}_2\text{O}(\text{g})$ using enthalpy of formation and absolute entropy data.

SOLUTION

$$\Delta \bar{g}_T^{\circ} = \Delta [\bar{h}(p_0, T) - T\bar{s}(p_0, T)] = \Delta \bar{h}(T) - T\Delta \bar{s}^{\circ}(T);$$

Handling the enthalpy term first and using Table G-1 we get,

$$\Delta \bar{h}(T) = \bar{h}_p(T) - \bar{h}_r(T) = \sum_p \nu_p \bar{h}_p(T) - \sum_r \nu_r \bar{h}_r(T);$$

$$\Rightarrow \Delta \bar{h}^{\circ} = \nu_{\text{CO}_2} \bar{h}_{f, \text{CO}_2} + \nu_{\text{H}_2\text{O}} \bar{h}_{f, \text{H}_2\text{O}} - \nu_{\text{CH}_4} \bar{h}_{f, \text{CH}_4} - \nu_{\text{O}_2} \bar{h}_{f, \text{O}_2};$$

$$\Rightarrow \Delta \bar{h}^{\circ} = (1)(-393,520) + (2)(-241,820) - (1)(-74,850) - (2)(0);$$

$$\Rightarrow \Delta \bar{h}^{\circ} = -802,310 \frac{\text{kJ}}{\text{kmol}}$$

Evaluating entropy and using the IG tables:

$$\Delta \bar{s}^{\circ}(T) = \sum_p \nu_p \bar{s}_p^{\circ}(T) - \sum_r \nu_r \bar{s}_r^{\circ}(T);$$

$$\Rightarrow \Delta \bar{s}^{\circ} = \nu_{\text{CO}_2} \bar{s}_{\text{CO}_2@298\text{ K}}^{\circ} + \nu_{\text{H}_2\text{O}} \bar{s}_{\text{H}_2\text{O}@298\text{ K}}^{\circ} - \nu_{\text{CH}_4} \bar{s}_{\text{CH}_4@298\text{ K}}^{\circ} - \nu_{\text{O}_2} \bar{s}_{\text{O}_2@298\text{ K}}^{\circ};$$

$$\Rightarrow \Delta \bar{s}^{\circ} = (1)(213.8) + (2)(188.83) - (1)(186.16) - (2)(205.04);$$

$$\Rightarrow \Delta \bar{s}^{\circ} = -4.78 \frac{\text{kJ}}{\text{kmol} \cdot \text{K}}$$

Combining all the terms now we obtain,

$$\Delta \bar{g}_T^{\circ} = \Delta \bar{h}(T) - T\Delta \bar{s}^{\circ}(T);$$

$$\Rightarrow \Delta \bar{g}_T^{\circ} = -802310 - (298)(-4.78);$$

$$\Rightarrow \Delta \bar{g}_T^{\circ} = -800,886 \frac{\text{kJ}}{\text{kmol}}$$

14-3-13 [BBN] Calculate the equilibrium constant (K) for $\text{CO}_2 \rightleftharpoons \text{CO} + 1/2\text{O}_2$ at (a) 500 K and (b) 1000 K.

SOLUTION



(a) At $T = 500$ K

Handling the enthalpy term first and using Table G-1 we get,

$$\Delta \bar{h}(T) = \bar{h}_p(T) - \bar{h}_r(T) = \sum_p \nu_p \bar{h}_p(T) - \sum_r \nu_r \bar{h}_r(T);$$

$$\begin{aligned} \Delta \bar{h}^0 &= \nu_{\text{CO}} (\bar{h}_{f,\text{CO}} + \Delta \bar{h}_{\text{CO}}(T)) + \nu_{\text{O}_2} (\bar{h}_{f,\text{O}_2} + \Delta \bar{h}_{\text{O}_2}(T)) - \nu_{\text{CO}_2} (\bar{h}_{f,\text{CO}_2} + \Delta \bar{h}_{\text{CO}_2}(T)); \\ \Rightarrow \Delta \bar{h}^0 &= (1)(-110,527 + 5,931) + (0.5)(0 + 6,088) - (1)(-393,522 + 8,314); \\ \Rightarrow \Delta \bar{h}^0 &= 283,656 \frac{\text{kJ}}{\text{kmol}} \end{aligned}$$

And then evaluating entropy and using the IG tables:

$$\begin{aligned} \Delta \bar{s}^0(T) &= \sum_p \nu_p \bar{s}_p^0(T) - \sum_r \nu_r \bar{s}_r^0(T); \\ \Rightarrow \Delta \bar{s}^0 &= \nu_{\text{CO}} \bar{s}_{\text{CO}@500\text{ K}}^0 + \nu_{\text{O}_2} \bar{s}_{\text{O}_2@500\text{ K}}^0 - \nu_{\text{CO}_2} \bar{s}_{\text{CO}_2@500\text{ K}}^0; \\ \Rightarrow \Delta \bar{s}^0 &= (1)(212.719) + (0.5)(220.589) - (1)(234.814); \\ \Rightarrow \Delta \bar{s}^0 &= 88.1995 \frac{\text{kJ}}{\text{kmol} \cdot \text{K}} \end{aligned}$$

Combining all the terms now we obtain,

$$\begin{aligned} \Delta \bar{g}_T^0 &= \Delta \bar{h}(T) - T \Delta \bar{s}^0(T); \\ \Rightarrow \Delta \bar{g}_T^0 &= 283,656 - (500)(88.1995); \\ \Rightarrow \Delta \bar{g}_T^0 &= 239,556.25 \frac{\text{kJ}}{\text{kmol}} \end{aligned}$$

$$\begin{aligned} \ln K &= -\frac{\Delta \bar{g}_T^0}{RT}; \\ \Rightarrow \ln K &= -\frac{239,556.25}{(8.314)(500)}; \\ \Rightarrow \ln K &= -57.627 \end{aligned}$$

(b) At $T = 1000$ K

Handling the enthalpy term first and using Table G-1 we get,

$$\Delta \bar{h}(T) = \bar{h}_p(T) - \bar{h}_r(T) = \sum_p \nu_p \bar{h}_p(T) - \sum_r \nu_r \bar{h}_r(T);$$

$$\Delta \bar{h}^\circ = \nu_{\text{CO}} (\bar{h}_{f,\text{CO}} + \Delta \bar{h}_{\text{CO}}(T)) + \nu_{\text{O}_2} (\bar{h}_{f,\text{O}_2} + \Delta \bar{h}_{\text{O}_2}(T)) - \nu_{\text{CO}_2} (\bar{h}_{f,\text{CO}_2} + \Delta \bar{h}_{\text{CO}_2}(T));$$

$$\Rightarrow \Delta \bar{h}^\circ = (1)(-110,527 + 21,686) + (0.5)(0 + 22,714) - (1)(-393,522 + 33,432);$$

$$\Rightarrow \Delta \bar{h}^\circ = 282,606 \frac{\text{kJ}}{\text{kmol}}$$

And then evaluating entropy and using the IG tables:

$$\Delta \bar{s}^\circ(T) = \sum_p \nu_p \bar{s}_p^\circ(T) - \sum_r \nu_r \bar{s}_r^\circ(T);$$

$$\Rightarrow \Delta \bar{s}^\circ = \nu_{\text{CO}} \bar{s}_{\text{CO}@1000\text{ K}}^\circ + \nu_{\text{O}_2} \bar{s}_{\text{O}_2@1000\text{ K}}^\circ - \nu_{\text{CO}_2} \bar{s}_{\text{CO}_2@1000\text{ K}}^\circ;$$

$$\Rightarrow \Delta \bar{s}^\circ = (1)(234.421) + (0.5)(243.634) - (1)(269.215);$$

$$\Rightarrow \Delta \bar{s}^\circ = 87.023 \frac{\text{kJ}}{\text{kmol} \cdot \text{K}}$$

Combining all the terms now we obtain,

$$\Delta \bar{g}_T^\circ = \Delta \bar{h}(T) - T \Delta \bar{s}^\circ(T);$$

$$\Rightarrow \Delta \bar{g}_T^\circ = 282,606 - (1000)(87.023);$$

$$\Rightarrow \Delta \bar{g}_T^\circ = 195,583 \frac{\text{kJ}}{\text{kmol}}$$

$$\ln K = -\frac{\Delta \bar{g}_T^\circ}{RT};$$

$$\Rightarrow \ln K = -\frac{195,583}{(8.314)(1000)};$$

$$\Rightarrow \ln K = -23.52$$

14-3-14 [BBE] One kmol of CO_2 is heated at a constant pressure of 100 kPa to 3000 K. (a) Calculate the equilibrium composition of CO_2 and use the IGE system state TESTcalc to verify your answers. (b) Use the n-IG system state TESTcalc and calculate the Gibbs function of the mixture $(1-x)\text{CO}_2 + x\text{CO} + (x/2)\text{O}_2$ at 100 kPa, 3000 K for x varying from 0 to 1. Show that for $x = 0.438$, Gibbs function reaches a minimum.

SOLUTION



Molar analysis:



$$\text{C}: 1 = 1 - \varepsilon + \varepsilon = 1$$

$$\text{O}: 2 = 2(1 - \varepsilon) + \varepsilon + 2a; \quad \Rightarrow 2 = 2 - 2\varepsilon + \varepsilon + 2a; \quad \Rightarrow a = \frac{\varepsilon}{2}$$

Therefore,

$$a + b + c = a + 1 - a + \frac{1 - a}{2} = \frac{3 - a}{2}$$

$$y_{\text{CO}_2} = \frac{1 - \varepsilon}{1 + a}; \quad y_{\text{CO}} = \frac{\varepsilon}{1 + a}; \quad y_{\text{O}_2} = \frac{a}{1 + a};$$

For $\text{CO}_2 \rightleftharpoons \text{CO} + 0.5\text{O}_2$ on Table G-3 at 3000 K, $\ln K_p = -1.111$

$$\ln K_p = \ln \left[\left(\frac{y_{\text{CO}}^{\nu_{\text{CO}}} y_{\text{O}_2}^{\nu_{\text{O}_2}}}{y_{\text{CO}_2}^{\nu_{\text{CO}_2}}} \right) \left(\frac{p}{p_0} \right)^{\nu_{\text{CO}} + \nu_{\text{O}_2} - \nu_{\text{CO}_2}} \right] = \ln \left[\frac{y_{\text{CO}}^1 y_{\text{O}_2}^{0.5}}{y_{\text{CO}_2}^1} \times (1)^{1.5-1} \right] = \ln \left[\frac{\left(\frac{\varepsilon}{1+a} \right) \left(\frac{a}{1+a} \right)^{0.5}}{\left(\frac{1-\varepsilon}{1+a} \right)} \right];$$

$$\Rightarrow \ln K_p = \ln \left[\left(\frac{\varepsilon}{1-\varepsilon} \right) \left(\frac{a}{1+a} \right)^{0.5} \right]; \quad \Rightarrow -1.111 = \ln \left[\left(\frac{\varepsilon}{1-\varepsilon} \right) \left(\frac{\varepsilon}{2+\varepsilon} \right)^{0.5} \right];$$

$$\Rightarrow e^{-1.111} = \left[\left(\frac{\varepsilon}{1-\varepsilon} \right) \left(\frac{\varepsilon}{2+\varepsilon} \right)^{0.5} \right] \quad \Rightarrow 0.3292296 = \left[\left(\frac{\varepsilon}{1-\varepsilon} \right) \left(\frac{\varepsilon}{2+\varepsilon} \right)^{0.5} \right];$$

$$\Rightarrow 0.1083921077 = \left[\left(\frac{\varepsilon}{1-\varepsilon} \right) \left(\frac{\varepsilon}{2+\varepsilon} \right)^{0.5} \right]^2; \quad \Rightarrow 0.1083921077 = \frac{\varepsilon^3}{\varepsilon^3 - 3\varepsilon + 2};$$

$$\Rightarrow 0.1083921077\varepsilon^3 - 0.3251763231\varepsilon + 0.2167843154 = \varepsilon^3;$$

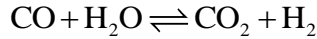
$$\Rightarrow 0 = 0.8916078923\varepsilon^3 + 0.3251763231\varepsilon - 0.2167843154;$$

$$\Rightarrow \varepsilon = 0.437328$$

$$\text{CO}_2 = 1 - \varepsilon = \mathbf{0.562672 \text{ kmol}}$$

14-3-15 [BBI] Calculate the equilibrium constant (K) for the water-gas reaction $\text{CO} + \text{H}_2\text{O}(\text{g}) \leftrightarrow \text{CO}_2 + \text{H}_2$ at (a) 298 K and (b) 1000 K.

SOLUTION



(a) Handling the enthalpy term first and using Table G-1 we get,

$$\begin{aligned}\Delta \bar{h}(T) &= \bar{h}_p(T) - \bar{h}_r(T) = \sum_p \nu_p \bar{h}_p(T) - \sum_r \nu_r \bar{h}_r(T); \\ \Rightarrow \Delta \bar{h}^\circ &= \nu_{\text{CO}_2} \bar{h}_{f,\text{CO}_2} + \nu_{\text{H}_2} \bar{h}_{f,\text{H}_2} - \nu_{\text{CO}} \bar{h}_{f,\text{CO}} - \nu_{\text{H}_2\text{O}} \bar{h}_{f,\text{H}_2\text{O}}; \\ \Rightarrow \Delta \bar{h}^\circ &= (1)(-393,520) + (1)(0) - (1)(-110,530) - (1)(-241,820); \\ \Rightarrow \Delta \bar{h}^\circ &= -41,170 \frac{\text{kJ}}{\text{kmol}}\end{aligned}$$

And then evaluating entropy and using the IG tables:

$$\begin{aligned}\Delta \bar{s}^\circ(T) &= \sum_p \nu_p \bar{s}_p^\circ(T) - \sum_r \nu_r \bar{s}_r^\circ(T); \\ \Rightarrow \Delta \bar{s}^\circ &= \nu_{\text{CO}_2} \bar{s}_{\text{CO}_2@298\text{ K}}^\circ + \nu_{\text{H}_2} \bar{s}_{\text{H}_2@298\text{ K}}^\circ - \nu_{\text{CO}} \bar{s}_{\text{CO@298 K}}^\circ - \nu_{\text{H}_2\text{O}} \bar{s}_{\text{H}_2\text{O@298 K}}^\circ; \\ \Rightarrow \Delta \bar{s}^\circ &= (1)(213.8) + (1)(130.68) - (1)(197.65) - (1)(188.83); \\ \Rightarrow \Delta \bar{s}^\circ &= -42 \frac{\text{kJ}}{\text{kmol} \cdot \text{K}}\end{aligned}$$

Combining all the terms now we obtain,

$$\begin{aligned}\Delta \bar{g}_T^\circ &= \Delta \bar{h}(T) - T \Delta \bar{s}^\circ(T); \\ \Rightarrow \Delta \bar{g}_T^\circ &= -41,170 - (298)(-42); \\ \Rightarrow \Delta \bar{g}_T^\circ &= -28,654 \frac{\text{kJ}}{\text{kmol}}\end{aligned}$$

$$\begin{aligned}\ln K &= -\frac{\Delta \bar{g}_T^\circ}{RT}; \\ \Rightarrow \ln K &= -\frac{-28,654}{(8.314)(298)}; \\ \Rightarrow \ln K &= 11.57 \\ \Rightarrow K &= 105,873\end{aligned}$$

(b) Handling the enthalpy term first and using Table G-1 we get,

$$\begin{aligned}\Delta \bar{h}(T) &= \bar{h}_p(T) - \bar{h}_r(T) = \sum_p \nu_p \bar{h}_p(T) - \sum_r \nu_r \bar{h}_r(T); \\ \Delta \bar{h}^\circ &= \nu_{\text{CO}_2} (\bar{h}_{f,\text{CO}_2} + \Delta \bar{h}_{\text{CO}_2}(T)) + \nu_{\text{H}_2} (\bar{h}_{f,\text{H}_2} + \Delta \bar{h}_{\text{H}_2}(T)) - \nu_{\text{CO}} (\bar{h}_{f,\text{CO}} + \Delta \bar{h}_{\text{CO}}(T)) - \nu_{\text{H}_2\text{O}} (\bar{h}_{f,\text{H}_2\text{O}} + \Delta \bar{h}_{\text{H}_2\text{O}}(T));\end{aligned}$$

$$\Rightarrow \Delta \bar{h}^{\circ} = (1)(-393,520 + 33,432) + (1)(20,686) - (1)(-110,530 + 21,686) - (1)(-241,820 + 25,978);$$

$$\Rightarrow \Delta \bar{h}^{\circ} = -34,716 \frac{\text{kJ}}{\text{kmol}}$$

And then evaluating entropy and using the IG tables:

$$\Delta \bar{s}^{\circ}(T) = \sum_p \nu_p \bar{s}_p^{\circ}(T) - \sum_r \nu_r \bar{s}_r^{\circ}(T);$$

$$\Rightarrow \Delta \bar{s}^{\circ} = \nu_{\text{CO}_2} \bar{s}_{\text{CO}_2@1000\text{ K}}^{\circ} + \nu_{\text{H}_2} \bar{s}_{\text{H}_2@1000\text{ K}}^{\circ} - \nu_{\text{CO}} \bar{s}_{\text{CO@1000 K}}^{\circ} - \nu_{\text{H}_2\text{O}} \bar{s}_{\text{H}_2\text{O@1000 K}}^{\circ};$$

$$\Rightarrow \Delta \bar{s}^{\circ} = (1)(269.215) + (1)(166.114) - (1)(234.421) - (1)(232.597);$$

$$\Rightarrow \Delta \bar{s}^{\circ} = -31.689 \frac{\text{kJ}}{\text{kmol} \cdot \text{K}}$$

Combining all the terms now we obtain,

$$\Delta \bar{g}_T^{\circ} = \Delta \bar{h}(T) - T \Delta \bar{s}^{\circ}(T);$$

$$\Rightarrow \Delta \bar{g}_T^{\circ} = -34,716 - (1000)(-31.689);$$

$$\Rightarrow \Delta \bar{g}_T^{\circ} = -3,027 \frac{\text{kJ}}{\text{kmol}}$$

$$\ln K = -\frac{\Delta \bar{g}_T^{\circ}}{RT};$$

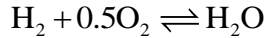
$$\Rightarrow \ln K = -\frac{-3,027}{(8.314)(1000)};$$

$$\Rightarrow \ln K = 0.364$$

$$\Rightarrow K = 1.44$$

14-3-16 [BBZ] Determine the equilibrium constant (K) for the reaction $\text{H}_2 + 1/2\text{O}_2 \leftrightarrow \text{H}_2\text{O}$ at (a) 298 K and (b) 2500 K.

SOLUTION



(a) At $T = 298 \text{ K}$

Handling the enthalpy term first and using Table G-1 we get,

$$\begin{aligned}\Delta \bar{h}(T) &= \bar{h}_p(T) - \bar{h}_r(T) = \sum_p \nu_p \bar{h}_p(T) - \sum_r \nu_r \bar{h}_r(T); \\ \Rightarrow \Delta \bar{h}^0 &= \nu_{\text{H}_2\text{O}} \bar{h}_{f,\text{H}_2\text{O}} - \nu_{\text{H}_2} \bar{h}_{f,\text{H}_2} - \nu_{\text{O}_2} \bar{h}_{f,\text{O}_2}; \\ \Rightarrow \Delta \bar{h}^0 &= (1)(-241,826) - (1)(0) - (0.5)(0); \\ \Rightarrow \Delta \bar{h}^0 &= -241,826 \frac{\text{kJ}}{\text{kmol}}\end{aligned}$$

And then evaluating entropy and using the IG tables:

$$\begin{aligned}\Delta \bar{s}^0(T) &= \sum_p \nu_p \bar{s}_p^0(T) - \sum_r \nu_r \bar{s}_r^0(T); \\ \Rightarrow \Delta \bar{s}^0 &= \nu_{\text{H}_2\text{O}} \bar{s}_{\text{H}_2\text{O}@298 \text{ K}}^0 - \nu_{\text{H}_2} \bar{s}_{\text{H}_2@298 \text{ K}}^0 - \nu_{\text{O}_2} \bar{s}_{\text{O}_2@298 \text{ K}}^0; \\ \Rightarrow \Delta \bar{s}^0 &= (1)(188.72) - (1)(130.574) - (0.5)(205.033); \\ \Rightarrow \Delta \bar{s}^0 &= -44.3705 \frac{\text{kJ}}{\text{kmol} \cdot \text{K}}\end{aligned}$$

Combining all the terms now we obtain,

$$\begin{aligned}\Delta \bar{g}_T^0 &= \Delta \bar{h}(T) - T \Delta \bar{s}^0(T); \\ \Rightarrow \Delta \bar{g}_T^0 &= -241,826 - (298)(-44.3705); \\ \Rightarrow \Delta \bar{g}_T^0 &= -228,603.59 \frac{\text{kJ}}{\text{kmol}}\end{aligned}$$

$$\begin{aligned}\ln K &= -\frac{\Delta \bar{g}_T^0}{RT}; \\ \Rightarrow \ln K &= -\frac{-228,603.59}{(8.314)(298)}; \\ \Rightarrow \ln K &= 92.27 \\ \Rightarrow K &= e^{92.27} = 1.18 \times 10^{40}\end{aligned}$$

(b) At $T = 2500 \text{ K}$

Handling the enthalpy term first and using Table G-1 we get,

$$\Delta \bar{h}(T) = \bar{h}_p(T) - \bar{h}_r(T) = \sum_p \nu_p \bar{h}_p(T) - \sum_r \nu_r \bar{h}_r(T);$$

$$\Delta \bar{h}^\circ = \nu_{\text{H}_2\text{O}} (\bar{h}_{f,\text{H}_2\text{O}} + \Delta \bar{h}_{\text{H}_2\text{O}}(T)) - \nu_{\text{H}_2} (\bar{h}_{f,\text{H}_2} + \Delta \bar{h}_{\text{H}_2}(T)) - \nu_{\text{O}_2} (\bar{h}_{f,\text{O}_2} + \Delta \bar{h}_{\text{O}_2}(T));$$

$$\Rightarrow \Delta \bar{h}^\circ = (1)(-241,826 + 98,964) - (1)(0 + 70,492) - (0.5)(0 + 78,375);$$

$$\Rightarrow \Delta \bar{h}^\circ = -252,541.5 \frac{\text{kJ}}{\text{kmol}}$$

And then evaluating entropy and using the IG tables:

$$\Delta \bar{s}^\circ(T) = \sum_p \nu_p \bar{s}_p^\circ(T) - \sum_r \nu_r \bar{s}_r^\circ(T);$$

$$\Rightarrow \Delta \bar{s}^\circ = \nu_{\text{H}_2\text{O}} \bar{s}_{\text{H}_2\text{O}@2500\text{K}}^\circ - \nu_{\text{H}_2} \bar{s}_{\text{H}_2@2500\text{K}}^\circ - \nu_{\text{O}_2} \bar{s}_{\text{O}_2@2500\text{K}}^\circ;$$

$$\Rightarrow \Delta \bar{s}^\circ = (1)(276.286) - (1)(196.125) - (0.5)(277.207);$$

$$\Rightarrow \Delta \bar{s}^\circ = -58.4425 \frac{\text{kJ}}{\text{kmol} \cdot \text{K}}$$

Combining all the terms now we obtain,

$$\Delta \bar{g}_T^\circ = \Delta \bar{h}(T) - T \Delta \bar{s}^\circ(T);$$

$$\Rightarrow \Delta \bar{g}_T^\circ = -252,541.5 - (2500)(-58.4425);$$

$$\Rightarrow \Delta \bar{g}_T^\circ = -106,435.25 \frac{\text{kJ}}{\text{kmol}}$$

$$\ln K = -\frac{\Delta \bar{g}_T^\circ}{RT};$$

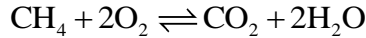
$$\Rightarrow \ln K = -\frac{-106,435.25}{(8.314)(2500)};$$

$$\Rightarrow \ln K = 5.12$$

$$\Rightarrow K = 167.34$$

14-3-17 [BBL] Determine the equilibrium constant (K) for the reaction $\text{CH}_4 + 2\text{O}_2 \leftrightarrow \text{CO}_2 + 2\text{H}_2\text{O}$ at 25°C .

SOLUTION



Handling the enthalpy term first and using Table G-1 we get,

$$\begin{aligned}\Delta \bar{h}(T) &= \bar{h}_p(T) - \bar{h}_r(T) = \sum_p \nu_p \bar{h}_p(T) - \sum_r \nu_r \bar{h}_r(T); \\ \Rightarrow \Delta \bar{h}^\circ &= \nu_{\text{CO}_2} \bar{h}_{f,\text{CO}_2} + \nu_{\text{H}_2\text{O}} \bar{h}_{f,\text{H}_2\text{O}} - \nu_{\text{CH}_4} \bar{h}_{f,\text{CH}_4} - \nu_{\text{O}_2} \bar{h}_{f,\text{O}_2}; \\ \Rightarrow \Delta \bar{h}^\circ &= (1)(-393,520) + (2)(-241,820) - (1)(-74,850) - (2)(0); \\ \Rightarrow \Delta \bar{h}^\circ &= -802,310 \frac{\text{kJ}}{\text{kmol}}\end{aligned}$$

And then evaluating entropy and using the IG tables:

$$\begin{aligned}\Delta \bar{s}^\circ(T) &= \sum_p \nu_p \bar{s}_p^\circ(T) - \sum_r \nu_r \bar{s}_r^\circ(T); \\ \Rightarrow \Delta \bar{s}^\circ &= \nu_{\text{CO}_2} \bar{s}_{\text{CO}_2@298\text{K}}^\circ + \nu_{\text{H}_2\text{O}} \bar{s}_{\text{H}_2\text{O}@298\text{K}}^\circ - \nu_{\text{CH}_4} \bar{s}_{\text{CH}_4@298\text{K}}^\circ - \nu_{\text{O}_2} \bar{s}_{\text{O}_2@298\text{K}}^\circ; \\ \Rightarrow \Delta \bar{s}^\circ &= (1)(213.8) + (2)(188.83) - (1)(186.16) - (2)(205.04); \\ \Rightarrow \Delta \bar{s}^\circ &= -4.78 \frac{\text{kJ}}{\text{kmol} \cdot \text{K}}\end{aligned}$$

Combining all the terms now we obtain,

$$\begin{aligned}\Delta \bar{g}_T^\circ &= \Delta \bar{h}(T) - T \Delta \bar{s}^\circ(T); \\ \Rightarrow \Delta \bar{g}_T^\circ &= -802,310 - (298)(-4.78); \\ \Rightarrow \Delta \bar{g}_T^\circ &= -800,885.56 \frac{\text{kJ}}{\text{kmol}}\end{aligned}$$

$$\begin{aligned}\ln K &= -\frac{\Delta \bar{g}_T^\circ}{RT}; \\ \Rightarrow \ln K &= -\frac{-800,885.56}{(8.314)(298)}; \\ \Rightarrow \ln K &= 323.25 \\ \Rightarrow K &= e^{323.25} = 2.43 \times 10^{140}\end{aligned}$$

14-3-18 [BBG] Determine the equilibrium constant (K) for the dissociation process $\text{CO}_2 \leftrightarrow \text{CO} + 1/2\text{O}_2$ at (a) 298 K and (b) 2000 K.

SOLUTION



(a) At $T = 298 \text{ K}$

Handling the enthalpy term first and using Table G-1 we get,

$$\begin{aligned}\Delta \bar{h}(T) &= \bar{h}_p(T) - \bar{h}_r(T) = \sum_p \nu_p \bar{h}_p(T) - \sum_r \nu_r \bar{h}_r(T); \\ \Rightarrow \Delta \bar{h}^\circ &= \nu_{\text{CO}} \bar{h}_{f,\text{CO}} + \nu_{\text{O}_2} \bar{h}_{f,\text{O}_2} - \nu_{\text{CO}_2} \bar{h}_{f,\text{CO}_2}; \\ \Rightarrow \Delta \bar{h}^\circ &= (1)(-110,530) + (0.5)(0) - (1)(-393,520); \\ \Rightarrow \Delta \bar{h}^\circ &= 282,990 \frac{\text{kJ}}{\text{kmol}}\end{aligned}$$

And then evaluating entropy and using the IG tables:

$$\begin{aligned}\Delta \bar{s}^\circ(T) &= \sum_p \nu_p \bar{s}_p^\circ(T) - \sum_r \nu_r \bar{s}_r^\circ(T); \\ \Rightarrow \Delta \bar{s}^\circ &= \nu_{\text{CO}} \bar{s}_{\text{CO}@298\text{K}}^\circ + \nu_{\text{O}_2} \bar{s}_{\text{O}_2@298\text{K}}^\circ - \nu_{\text{CO}_2} \bar{s}_{\text{CO}_2@298\text{K}}^\circ; \\ \Rightarrow \Delta \bar{s}^\circ &= (1)(197.543) + (0.5)(205.033) - (1)(213.685); \\ \Rightarrow \Delta \bar{s}^\circ &= 86.3745 \frac{\text{kJ}}{\text{kmol} \cdot \text{K}}\end{aligned}$$

Combining all the terms now we obtain,

$$\begin{aligned}\Delta \bar{g}_T^\circ &= \Delta \bar{h}(T) - T \Delta \bar{s}^\circ(T); \\ \Rightarrow \Delta \bar{g}_T^\circ &= 282,990 - (298)(86.3745); \\ \Rightarrow \Delta \bar{g}_T^\circ &= 257,250.399 \frac{\text{kJ}}{\text{kmol}}\end{aligned}$$

$$\begin{aligned}\ln K &= -\frac{\Delta \bar{g}_T^\circ}{RT}; \\ \Rightarrow \ln K &= -\frac{257,250.399}{(8.314)(298)}; \\ \Rightarrow \ln K &= -103.83\end{aligned}$$

(b) At $T = 2000 \text{ K}$

Handling the enthalpy term first and using Table G-1 we get,

$$\Delta \bar{h}(T) = \bar{h}_p(T) - \bar{h}_r(T) = \sum_p \nu_p \bar{h}_p(T) - \sum_r \nu_r \bar{h}_r(T);$$

$$\begin{aligned}\Delta \bar{h}^{\circ} &= \nu_{\text{CO}} (\bar{h}_{f,\text{CO}} + \Delta \bar{h}_{\text{CO}}(T)) + \nu_{\text{O}_2} (\bar{h}_{f,\text{O}_2} + \Delta \bar{h}_{\text{O}_2}(T)) - \nu_{\text{CO}_2} (\bar{h}_{f,\text{CO}_2} + \Delta \bar{h}_{\text{CO}_2}(T)); \\ \Rightarrow \Delta \bar{h}^{\circ} &= (1)(-110,530 + 56,739) + (0.5)(0 + 59,199) - (1)(-393,520 + 91,440); \\ \Rightarrow \Delta \bar{h}^{\circ} &= 277,888.5 \frac{\text{kJ}}{\text{kmol}}\end{aligned}$$

And then evaluating entropy and using the IG tables:

$$\begin{aligned}\Delta \bar{s}^{\circ}(T) &= \sum_p \nu_p \bar{s}_p^{\circ}(T) - \sum_r \nu_r \bar{s}_r^{\circ}(T); \\ \Rightarrow \Delta \bar{s}^{\circ} &= \nu_{\text{CO}} \bar{s}_{\text{CO}@2000\text{K}}^{\circ} + \nu_{\text{O}_2} \bar{s}_{\text{O}_2@2000\text{K}}^{\circ} - \nu_{\text{CO}_2} \bar{s}_{\text{CO}_2@2000\text{K}}^{\circ}; \\ \Rightarrow \Delta \bar{s}^{\circ} &= (1)(258.6) + (0.5)(268.655) - (1)(309.21); \\ \Rightarrow \Delta \bar{s}^{\circ} &= 83.7175 \frac{\text{kJ}}{\text{kmol} \cdot \text{K}}\end{aligned}$$

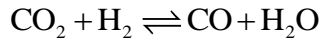
Combining all the terms now we obtain,

$$\begin{aligned}\Delta \bar{g}_T^{\circ} &= \Delta \bar{h}(T) - T \Delta \bar{s}^{\circ}(T); \\ \Rightarrow \Delta \bar{g}_T^{\circ} &= 277,888.5 - (2000)(83.7175); \\ \Rightarrow \Delta \bar{g}_T^{\circ} &= 110,453.5 \frac{\text{kJ}}{\text{kmol}}\end{aligned}$$

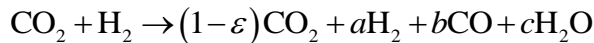
$$\begin{aligned}\ln K &= -\frac{\Delta \bar{g}_T^{\circ}}{RT}; \\ \Rightarrow \ln K &= -\frac{110,453.5}{(8.314)(2000)}; \\ \Rightarrow \ln K &= -6.64\end{aligned}$$

14-3-19 [BBK] For the chemical reaction $\text{CO}_2 + \text{H}_2 \leftrightarrow \text{CO} + \text{H}_2\text{O}$, the equilibrium value of the degree of reaction (forward completion fraction) at 1200 K is 0.56. Determine the equilibrium constant and the change in Gibbs function.

SOLUTION



Molar analysis:



$$\text{C}: 1 = (1-\varepsilon) + b; \quad \Rightarrow b = \varepsilon$$

$$\text{O}: 2 = 2(1-\varepsilon) + b + c; \quad \Rightarrow 2 = 2 - 2\varepsilon + \varepsilon + c; \quad \Rightarrow c = \varepsilon$$

$$\text{H}: 2 = 2a + 2c; \quad \Rightarrow 2 = 2a + 2\varepsilon; \quad \Rightarrow a = 1 - \varepsilon$$

Therefore,

$$(1-\varepsilon) + a + b + c = (1-\varepsilon) + (1-\varepsilon) + \varepsilon + \varepsilon = 2$$

$$y_{\text{CO}_2} = \frac{1-\varepsilon}{2} = 0.22; \quad y_{\text{H}_2} = \frac{a}{2} = \frac{1-\varepsilon}{2} = 0.22; \quad y_{\text{CO}} = \frac{b}{2} = \frac{\varepsilon}{2} = 0.28; \quad y_{\text{H}_2\text{O}} = \frac{c}{2} = \frac{\varepsilon}{2} = 0.28$$

$$\ln K_p = \ln \left[\left(\frac{y_{\text{CO}}^{\nu_{\text{CO}}} y_{\text{H}_2\text{O}}^{\nu_{\text{H}_2\text{O}}}}{y_{\text{CO}_2}^{\nu_{\text{CO}_2}} y_{\text{H}_2}^{\nu_{\text{H}_2}}} \right) \left(\frac{p}{p_0} \right)^{\nu_{\text{CO}} + \nu_{\text{H}_2\text{O}} - \nu_{\text{CO}_2} - \nu_{\text{H}_2}} \right] = \ln \left[\left(\frac{y_{\text{CO}}^1 y_{\text{H}_2\text{O}}^1}{y_{\text{CO}_2}^1 y_{\text{H}_2}^1} \right) \left(\frac{p}{p_0} \right)^{2-2} \right] = \ln \left[\frac{(0.28)(0.28)}{(0.22)(0.22)} \right];$$

$$\Rightarrow \ln K_p = \ln [1.6198];$$

$$\Rightarrow \ln K_p = 0.4823;$$

$$\Rightarrow K_p = 1.6198$$

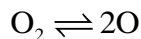
$$\ln K = -\frac{\Delta \bar{g}_T^0}{RT};$$

$$\Rightarrow \ln (1.6198) = -\frac{\Delta \bar{g}_T^0}{(8.314)(1200)};$$

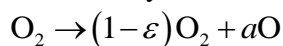
$$\Rightarrow \Delta \bar{g}_T^0 = 4812.05$$

14-3-20 [BBX] Determine the temperature at which 2% of diatomic oxygen (O_2) dissociates into monatomic oxygen (O) at a pressure of 3 atm.

SOLUTION



Molar analysis:



$$O: 2 = 2(1-\varepsilon) + a; \quad \Rightarrow a = 2\varepsilon$$

Therefore,

$$(1-\varepsilon) + a = 1 - \varepsilon + 2\varepsilon = 1 + \varepsilon$$

$$y_{O_2} = \frac{(1-\varepsilon)}{1+\varepsilon} = \frac{0.98}{1.02}; \quad y_O = \frac{2\varepsilon}{1+\varepsilon} = \frac{0.04}{1.02}$$

$$\ln K_p = \ln \left[\left(\frac{y_O^{v_O}}{y_{O_2}^{v_{O_2}}} \right) \left(\frac{p}{p_0} \right)^{v_O - v_{O_2}} \right] = \ln \left[\frac{y_O^2}{y_{O_2}} \times (3)^{2-1} \right] = \ln \left[\frac{\left(\frac{0.04}{1.02} \right)^2}{\left(\frac{0.98}{1.02} \right)} \times (3)^{2-1} \right] = \ln \left[\left(\frac{0.04}{1.02} \right)^2 \left(\frac{1.02}{0.98} \right) (3) \right];$$

$$\Rightarrow \ln K_p = \ln[0.048019]; \quad \Rightarrow \ln K = -5.338739;$$

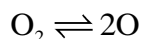
Looking at Table G-3:

Temperature \approx **2866 K**

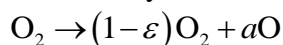
14-3-21 [BBP] Oxygen (O_2) is heated to 3000 K at a constant pressure of 5 atm. Determine the percentage of O_2 that will dissociate into O during this process.

SOLUTION

Given: $T = 3000 \text{ K}$; $p = 5 \text{ atm}$



Molar analysis:



$$O: 2 = 2(1-\varepsilon) + a; \quad \Rightarrow a = 2\varepsilon$$

Therefore,

$$(1-\varepsilon) + a = 1 - \varepsilon + 2\varepsilon = 1 + \varepsilon$$

$$y_{O_2} = \frac{(1-\varepsilon)}{1+\varepsilon}; \quad y_O = \frac{2\varepsilon}{1+\varepsilon}$$

For $O_2 \rightleftharpoons 2O$ in the $\ln K_p$ Table at 3000K, $\ln K_p = -4.357$

$$\begin{aligned} \ln K_p &= \ln \left[\left(\frac{y_O^{v_O}}{y_{O_2}^{v_{O_2}}} \right) \left(\frac{p}{p_0} \right)^{v_O - v_{O_2}} \right] = \ln \left[\left(\frac{y_O^2}{y_{O_2}} \right) (5)^{2-1} \right] = \ln \left[\frac{\left(\frac{2\varepsilon}{1+\varepsilon} \right)^2}{\left(\frac{1-\varepsilon}{1+\varepsilon} \right)} \times (5)^{2-1} \right] = \ln \left[\left(\frac{2\varepsilon}{1+\varepsilon} \right)^2 \left(\frac{1+\varepsilon}{1-\varepsilon} \right) (5) \right]; \\ \Rightarrow \ln K_p &= \ln \left[\frac{(5)(2\varepsilon)^2}{(1+\varepsilon)(1-\varepsilon)} \right] = \ln \left[\frac{20\varepsilon^2}{1-\varepsilon^2} \right]; \\ \Rightarrow -4.357 &= \ln \left[\frac{20\varepsilon^2}{1-\varepsilon^2} \right]; \quad \Rightarrow e^{-4.357} = \left[\frac{20\varepsilon^2}{1-\varepsilon^2} \right]; \\ \Rightarrow 0.012817 &= \left[\frac{20\varepsilon^2}{1-\varepsilon^2} \right]; \quad \Rightarrow 0.012817 - 0.012817\varepsilon^2 = 20\varepsilon^2 \\ \Rightarrow 20.012817\varepsilon^2 &= 0.012817; \quad \Rightarrow \varepsilon = 0.0253; \end{aligned}$$

Thus the percentage of O_2 that dissociates is **2.53%**.

14-3-22 [BBU] $\text{H}_2\text{O}(\text{g})$ dissociates into an equilibrium mixture at 3000 K and 100 kPa. Assume the equilibrium mixture consists of $\text{H}_2(\text{g})$, H_2O , O_2 , and OH , determine the equilibrium composition of (a) H_2O , (b) OH (in kmols).

SOLUTION

Given: $T = 3000 \text{ K}$; $p = 100 \text{ kPa}$

Molar analysis:

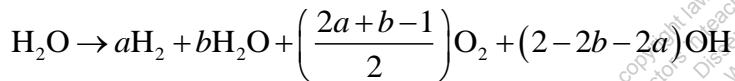


$$\text{H: } 2 = 2a + 2b + d \quad \Rightarrow d = 2 - 2b - 2a$$

$$\text{O: } 1 = b + 2c + d \quad \Rightarrow c = \frac{2a + b - 1}{2}$$

$$a + b + c + d = a + b + \frac{2a + b - 1}{2} + 2 - 2b - 2a = 1.5 - 0.5b$$

Plugging the relations for the stoichiometric coefficients into the equation above we get,



$$y_{\text{H}_2} = \frac{a}{1.5 - 0.5b}; \quad y_{\text{H}_2\text{O}} = \frac{b}{1.5 - 0.5b}; \quad y_{\text{O}_2} = \frac{2a + b - 1}{3 - b}; \quad y_{\text{OH}} = \frac{2 - 2b - 2a}{1.5 - 0.5b}$$

Now we utilize the equilibrium relations constants from Table G-3

$$\text{H}_2\text{O} \rightleftharpoons \text{H}_2 + \frac{1}{2}\text{O}_2; \quad \ln K_{p1@T=3000 \text{ K}} = -3.086$$

$$\text{H}_2\text{O} \rightleftharpoons \frac{1}{2}\text{H}_2 + \text{OH}; \quad \ln K_{p2@T=3000 \text{ K}} = -2.937$$

Now plugging in all the values into equation Eq. 14.53 to obtain

$$\begin{aligned} \ln K_{p1@T=3000 \text{ K}} &= \ln \left[\frac{\left(\frac{a}{1.5 - 0.5b}\right) \left(\frac{2a + b - 1}{3 - b}\right)^{\frac{1}{2}}}{\left(\frac{b}{1.5 - 0.5b}\right)} \right]; \quad \Rightarrow e^{-3.086} = \left(\frac{a}{b}\right) \left(\frac{2a + b - 1}{3 - b}\right)^{\frac{1}{2}}; \\ &\Rightarrow (e^{-3.086})^2 = \left[\left(\frac{a}{b}\right) \left(\frac{2a + b - 1}{3 - b}\right)^{\frac{1}{2}}\right]^2; \quad \Rightarrow (0.045684)^2 = \left(\frac{a^2}{b^2}\right) \left(\frac{2a + b - 1}{3 - b}\right); \\ &\Rightarrow 0.00208706 = \frac{2a^3 + ba^2 - a^2}{3b^2 - b^3} \end{aligned}$$

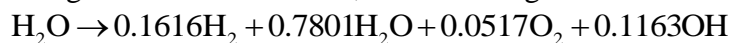
$$\ln K_{p_2} = \ln \left(\frac{\left(\frac{a}{1.5-0.5b} \right)^{\frac{1}{2}} \left(\frac{2-2b-2a}{1.5-0.5b} \right)}{\left(\frac{b}{1.5-0.5b} \right)} \right); \quad \Rightarrow e^{-2.937} = \left(\frac{2-2b-2a}{b} \right) \left(\frac{a}{1.5-0.5b} \right)^{\frac{1}{2}};$$

$$\Rightarrow (0.05302456)^2 = \left(\left(\frac{2-2b-2a}{b} \right) \left(\frac{a}{1.5-0.5b} \right)^{\frac{1}{2}} \right)^2;$$

$$\Rightarrow 0.002811604 = \left(\frac{a}{1.5-0.5b} \right) \left(\frac{4-8b-8a+8ab+4a^2+4b^2}{b^2} \right);$$

We now have two simultaneous equations to solve for a and b

Using the n-IGE TESTcalc, the following solution can be obtained:



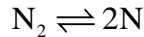
(a) $\text{H}_2\text{O} = 0.7801 \text{ kmol}$

(b) $\text{OH} = 0.1163 \text{ kmol}$

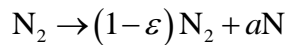
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14-3-23 [BBC] Nitrogen (N_2) is heated to 3000 K at a constant pressure of 5 atm. (a) Determine the percentage of N_2 that will dissociate into N during this process. What-if Scenario: What would the answer be if the conditions were (b) 5 atm, 5000 K and (c) 0.1 atm, 5000 K?

SOLUTION



Molar analysis:



$$N: 2 = 2(1-\varepsilon) + a; \quad \Rightarrow a = 2\varepsilon$$

Therefore,

$$(1-\varepsilon) + a = 1 - \varepsilon + 2\varepsilon = 1 + \varepsilon$$

$$y_{N_2} = \frac{1-\varepsilon}{1+\varepsilon}; \quad y_N = \frac{2\varepsilon}{1+\varepsilon}$$

(a) For $N_2 \rightleftharpoons 2N$ from Table G-3 at 3000K, $\ln K_p = -22.359$ and $p = 5$ atm

$$\ln K_p = \ln \left[\left(\frac{y_N^{v_N}}{y_{N_2}^{v_{N_2}}} \right) \left(\frac{5}{p_0} \right)^{v_N - v_{N_2}} \right] = \ln \left[\left(\frac{y_N^2}{y_{N_2}} \right) (5)^{2-1} \right] = \ln \left[\frac{\left(\frac{2\varepsilon}{1+\varepsilon} \right)^2}{\left(\frac{1-\varepsilon}{1+\varepsilon} \right)} \times (5)^{2-1} \right];$$

$$\Rightarrow \ln K_p = \ln \left[\frac{(5)(2\varepsilon)^2}{(1+\varepsilon)(1-\varepsilon)} \right] = \ln \left[\frac{20\varepsilon^2}{1-\varepsilon^2} \right];$$

$$\Rightarrow -22.359 = \ln \left[\frac{20\varepsilon^2}{1-\varepsilon^2} \right]; \quad \Rightarrow e^{-22.359} = \left[\frac{20\varepsilon^2}{1-\varepsilon^2} \right];$$

$$\Rightarrow 1.95 \times 10^{-10} = \left[\frac{20\varepsilon^2}{1-\varepsilon^2} \right]; \quad \Rightarrow 1.95 \times 10^{-10} - (1.95 \times 10^{-10})\varepsilon^2 = 20\varepsilon^2;$$

$$\Rightarrow 20\varepsilon^2 = 0; \quad \Rightarrow \varepsilon = 0$$

Thus **0%** of the N_2 dissociates.

(b) For $N_2 \rightleftharpoons 2N$ from Table G-3 at 5000 K, $\ln K_p = -6.807$ and at $p = 5$ atm

$$\ln K_p = \ln \left[\left(\frac{y_N^{v_N}}{y_{N_2}^{v_{N_2}}} \right) \left(\frac{5}{p_0} \right)^{v_N - v_{N_2}} \right] = \ln \left[\left(\frac{y_N^2}{y_{N_2}} \right) (5)^{2-1} \right] = \ln \left[\frac{\left(\frac{2\varepsilon}{1+\varepsilon} \right)^2}{\left(\frac{1-\varepsilon}{1+\varepsilon} \right)} \times (5)^{2-1} \right];$$

$$\Rightarrow \ln K_p = \ln \left[\frac{(5)(2\varepsilon)^2}{(1+\varepsilon)(1-\varepsilon)} \right] = \ln \left[\frac{20\varepsilon^2}{1-\varepsilon^2} \right];$$

$$\Rightarrow -6.807 = \ln \left[\frac{20\varepsilon^2}{1-\varepsilon^2} \right]; \quad \Rightarrow e^{-6.807} = \left[\frac{20\varepsilon^2}{1-\varepsilon^2} \right];$$

$$\Rightarrow 0.001106 = \left[\frac{20\varepsilon^2}{1-\varepsilon^2} \right]; \quad \Rightarrow 0.001106 - 0.001106\varepsilon^2 = 20\varepsilon^2;$$

$$\Rightarrow 20.001106\varepsilon^2 = 0.001106; \quad \Rightarrow a = 0.00744$$

Thus **0.74%** of the N_2 dissociates.

(c) For $N_2 \rightleftharpoons 2N$ from Table G-3 at 5000 K, $\ln K_p = -6.807$ and at $p = 0.1$ atm

$$\ln K_p = \ln \left[\left(\frac{y_N^{v_N}}{y_{N_2}^{v_{N_2}}} \right) \left(\frac{5}{p_0} \right)^{v_N - v_{N_2}} \right] = \ln \left[\left(\frac{y_N^2}{y_{N_2}} \right) (0.1)^{2-1} \right] = \ln \left[\frac{\left(\frac{2\varepsilon}{1+\varepsilon} \right)^2}{\left(\frac{1-\varepsilon}{1+\varepsilon} \right)} \times (0.1)^{2-1} \right];$$

$$\Rightarrow \ln K_p = \ln \left[\frac{(0.1)(2\varepsilon)^2}{(1+\varepsilon)(1-\varepsilon)} \right] = \ln \left[\frac{0.4\varepsilon^2}{1-\varepsilon^2} \right];$$

$$\Rightarrow -6.807 = \ln \left[\frac{0.4\varepsilon^2}{1-\varepsilon^2} \right]; \quad \Rightarrow e^{-6.807} = \left[\frac{0.4\varepsilon^2}{1-\varepsilon^2} \right];$$

$$\Rightarrow 0.001106 = \left[\frac{0.4\varepsilon^2}{1-\varepsilon^2} \right]; \quad \Rightarrow 0.001106 - 0.001106\varepsilon^2 = 0.4\varepsilon^2;$$

$$\Rightarrow 0.401106\varepsilon^2 = 0.001106; \quad \Rightarrow \varepsilon = 0.0525$$

Thus **5.25%** of the N_2 dissociates.

14-3-24 [BBV] Carbon dioxide (CO₂) is heated to 3200 K at a constant pressure of 2 atm. Determine the percentage of CO₂ that will dissociate into CO and O₂ during the process.

SOLUTION



Molar Analysis:



$$\text{C: } 1 = (1-\varepsilon) + a; \quad \Rightarrow a = \varepsilon$$

$$\text{O: } 2 = 2(1-\varepsilon) + a + 2b; \quad \Rightarrow b = \frac{\varepsilon}{2}$$

Therefore,

$$(1-\varepsilon) + a + b = 1 - \varepsilon + \varepsilon + \frac{\varepsilon}{2} = 1 + \frac{\varepsilon}{2} = \frac{2+\varepsilon}{2}$$

$$y_{\text{CO}_2} = \frac{1-\varepsilon}{\left(\frac{2+\varepsilon}{2}\right)} = \frac{2-2\varepsilon}{2+\varepsilon}; \quad y_{\text{CO}} = \frac{a}{\left(\frac{2+\varepsilon}{2}\right)} = \frac{2\varepsilon}{2+\varepsilon}; \quad y_{\text{O}_2} = \frac{b}{\left(\frac{2+\varepsilon}{2}\right)} = \frac{\varepsilon}{2+\varepsilon}$$

For $\text{CO}_2 \rightleftharpoons \text{CO} + \frac{1}{2}\text{O}_2$ from Table G-3, at 3200 K, $\ln K_p = -0.429$ and $p = 2$ atm

$$\ln K_p = \ln \left[\left(\frac{y_{\text{CO}}^{\nu_{\text{CO}}} y_{\text{O}_2}^{\nu_{\text{O}_2}}}{y_{\text{CO}_2}^{\nu_{\text{CO}_2}}} \right) \left(\frac{2}{p_0} \right)^{\nu_{\text{CO}} + \nu_{\text{O}_2} - \nu_{\text{CO}_2}} \right] = \ln \left[\left(\frac{\left(\frac{2\varepsilon}{2+\varepsilon} \right)^1 \left(\frac{\varepsilon}{2+\varepsilon} \right)^{0.5}}{\left(\frac{2-2\varepsilon}{2+\varepsilon} \right)^1} \right) (2)^{0.5} \right] = \ln \left[\left(\frac{2\varepsilon}{2-2\varepsilon} \right)^1 \left(\frac{\varepsilon}{2+\varepsilon} \right)^{0.5} \times (2)^{0.5} \right];$$

$$\Rightarrow -0.429 = \ln \left[\left(\frac{2\varepsilon}{2-2\varepsilon} \right)^1 \left(\frac{\varepsilon}{2+\varepsilon} \right)^{0.5} \times (2)^{0.5} \right]; \quad \Rightarrow e^{-0.429} = \left[\left(\frac{2\varepsilon}{2-2\varepsilon} \right)^1 \left(\frac{\varepsilon}{2+\varepsilon} \right)^{0.5} \times (2)^{0.5} \right];$$

$$\Rightarrow 0.6511599 = \left[\left(\frac{2\varepsilon}{2-2\varepsilon} \right)^1 \left(\frac{\varepsilon}{2+\varepsilon} \right)^{0.5} \times (2)^{0.5} \right]; \quad \Rightarrow 0.42400925 = \left[\left(\frac{2\varepsilon}{2-2\varepsilon} \right)^2 \left(\frac{\varepsilon}{2+\varepsilon} \right)^1 \times (2)^1 \right];$$

$$\Rightarrow 0.21200463 = \left[\frac{\varepsilon^3}{\varepsilon^3 - 3\varepsilon + 2} \right];$$

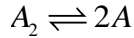
$$\Rightarrow 0.21200463\varepsilon^3 - 0.63601388\varepsilon + 0.42400925 = \varepsilon^3;$$

$$\Rightarrow 0.42400925 - 0.63601388\varepsilon - 0.78799537\varepsilon^3 = 0; \quad \Rightarrow \varepsilon = 0.506079$$

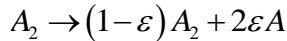
Thus **50.61%** of the CO₂ dissociates.

14-3-25 [BBQ] Consider the dissociation of 1 kmol of A_2 through the elementary step $A_2 \leftrightarrow 2A$. If ε stands for the degree of dissociation (fraction of A_2 by volume that is dissociated), the overall reaction can be represented by $A_2 \leftrightarrow (1-\varepsilon)A_2 + 2\varepsilon A$. At 500 K and 100 kPa, the equilibrium constant is calculated as 1. (a) Determine ε . (b) What would be the value of ε if the pressure is reduced to 0.01 kPa. (c) What-if Scenario: Plot how the degree of dissociation changes as the pressure is increased from 0.01 MPa to 1 MPa.

SOLUTION



Molar analysis:



Therefore.

$$(1-\varepsilon) + 2\varepsilon = 1 + \varepsilon$$

$$y_{A_2} = \frac{1-\varepsilon}{1+\varepsilon}; \quad y_A = \frac{2\varepsilon}{1+\varepsilon};$$

(a) For $A_2 \rightleftharpoons 2A$ at 500K and $p = 100 \text{ kPa}$, $K_p = 1$

$$K_p = \left[\left(\frac{y_A^{v_A}}{y_{A_2}^{v_{A_2}}} \right) \left(\frac{1}{p_0} \right)^{v_A - v_{A_2}} \right] = \left[\left(\frac{y_A^2}{y_{A_2}} \right) (1)^{2-1} \right] = \left[\frac{\left(\frac{2\varepsilon}{1+\varepsilon} \right)^2}{\left(\frac{1-\varepsilon}{1+\varepsilon} \right)} \right] = \left[\left(\frac{2\varepsilon}{1+\varepsilon} \right)^2 \left(\frac{1+\varepsilon}{1-\varepsilon} \right) \right] = \left[\frac{4\varepsilon^2}{1-\varepsilon^2} \right];$$

$$\Rightarrow 1 = \left[\frac{4\varepsilon^2}{1-\varepsilon^2} \right]; \quad \Rightarrow 1 - \varepsilon^2 = 4\varepsilon^2; \quad \Rightarrow 0 = 1 - 5\varepsilon^2;$$

$$\Rightarrow \varepsilon = 0.44721 = 44.77\%$$

(b) For $A_2 \rightleftharpoons 2A$ at 500 K and $p = 0.01 \text{ kPa}$, $K_p = 1$

$$K_p = \left[\left(\frac{y_A^{v_A}}{y_{A_2}^{v_{A_2}}} \right) \left(\frac{0.01}{p_0} \right)^{v_A - v_{A_2}} \right] = \left[\left(\frac{y_A^2}{y_{A_2}} \right) (0.0001)^{2-1} \right] = \left[\frac{\left(\frac{2\varepsilon}{1+\varepsilon} \right)^2}{\left(\frac{1-\varepsilon}{1+\varepsilon} \right)} \times (0.0001) \right] = \left[\left(\frac{2\varepsilon}{1+\varepsilon} \right)^2 \left(\frac{1+\varepsilon}{1-\varepsilon} \right) \times (0.0001) \right];$$

$$\Rightarrow K_p = \left[\frac{4\varepsilon^2}{1-\varepsilon^2} \times (0.0001) \right]; \quad \Rightarrow 1 = \left[\frac{4\varepsilon^2}{1-\varepsilon^2} \times (0.0001) \right]; \quad \Rightarrow 1 - \varepsilon^2 = 0.0004\varepsilon^2;$$

$$\Rightarrow 0 = 1 - 1.0004\varepsilon^2; \quad \Rightarrow \varepsilon = 0.99980006 = 99.98\%$$

(c) Plot how ε changes with pressure from 0.01 MPa to 1 MPa.

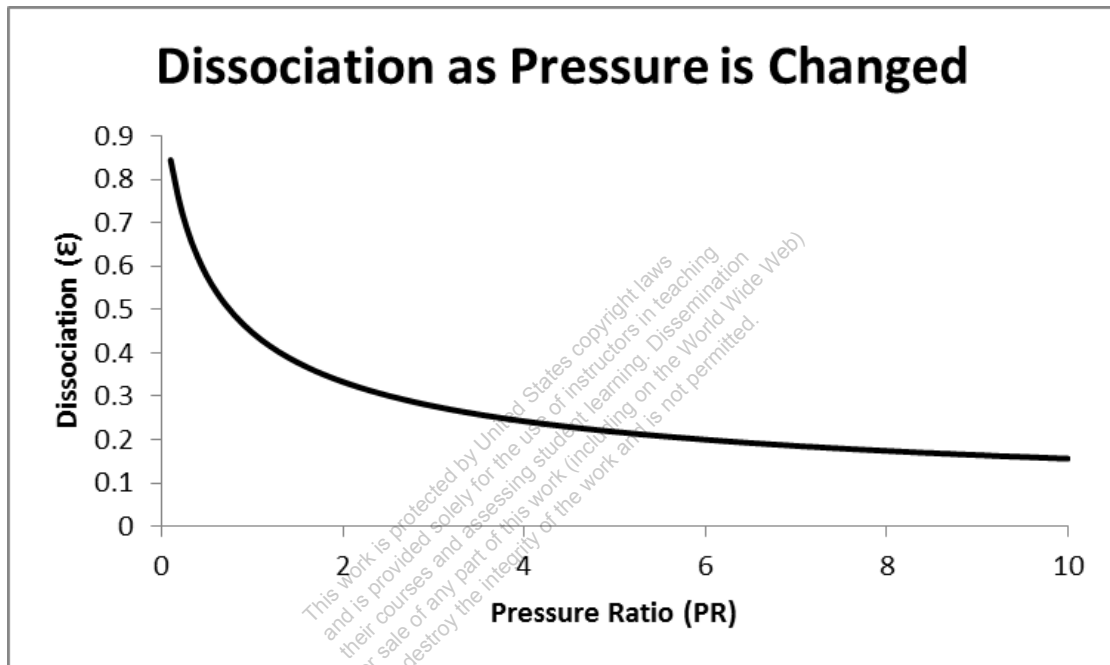
To solve this, we need to first solve the base equation:

$$1 = \frac{4\varepsilon^2}{1 - \varepsilon^2} \times PR$$

Where PR is the ratio of mixture pressure to ambient pressure. This simplifies to:

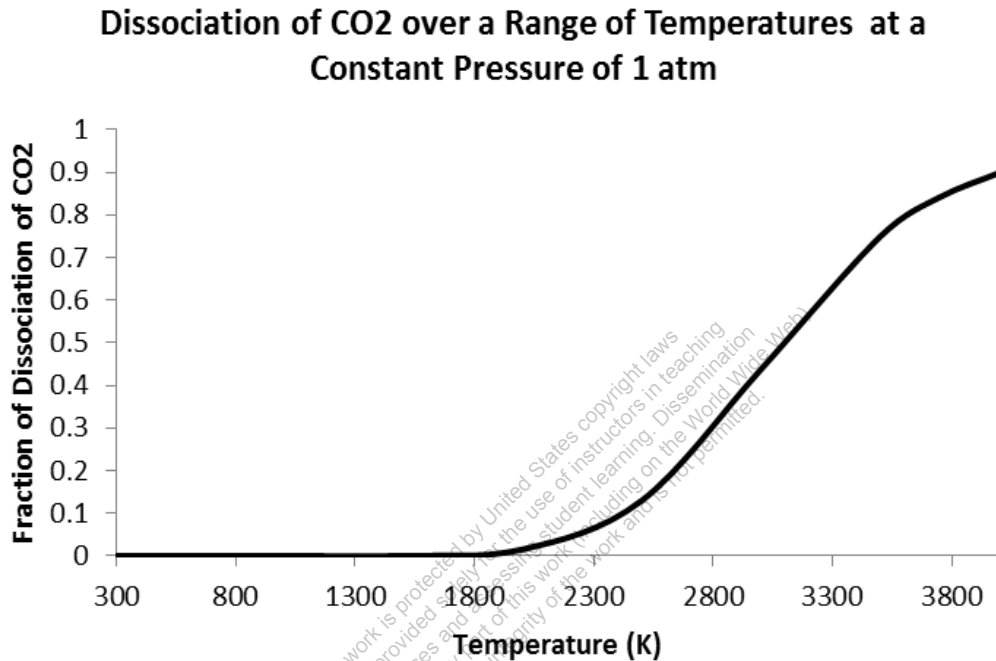
$$\varepsilon = \sqrt{\frac{1}{4PR + 1}}$$

When this relationship is plotted, we achieve the following graph:



14-3-26 [BBT] One kmol of carbon dioxide (CO_2) is heated from 300 K to 4000 K at a constant pressure of 1 atm. Use the IGE system state TESTcalc, set up the reactants as 1 kmol of CO_2 and select CO_2 , CO , and O_2 as the possible products. Now calculate a series of equilibrium products states (in the state panel, select the Products radio-button) for several temperatures ranging from 300 K through 3000 K. Plot how the fraction of CO_2 dissociated changes with temperature.

TEST Solution:



14-3-27 [BBY] A mixture of 1 kmol of CO and 2 kmol of O₂ is heated to 2000 K at a pressure of 2 atm. Determine the equilibrium composition of (a) O₂, (b) CO₂ (in kmols) assuming the mixture consists of CO₂, CO and O₂.

SOLUTION

Given: $T = 2000 \text{ K}$; $p = 2 \text{ atm}$

Molar Analysis:



$$\text{C: } 1 = a + b; \quad \Rightarrow b = 1 - a$$

$$\text{O: } 1 + 4 = 2a + b + 2c; \quad \Rightarrow c = \frac{4 - a}{2}$$

Therefore:

$$a + b + c = 1 + \frac{4 - a}{2}$$

$$y_{\text{CO}_2} = \frac{a}{1 + \frac{4 - a}{2}}; \quad y_{\text{CO}} = \frac{1 - a}{1 + \frac{4 - a}{2}}; \quad y_{\text{O}_2} = \frac{\frac{4 - a}{2}}{1 + \frac{4 - a}{2}}$$

For $\text{CO}_2 \rightleftharpoons \text{CO} + \frac{1}{2}\text{O}_2$ from Table G-3 at 2000 K, $\ln K = -6.635$ and $p = 2 \text{ atm}$

$$\ln K_p = \ln \left[\left(\frac{y_{\text{CO}}^{\nu_{\text{CO}}} y_{\text{O}_2}^{\nu_{\text{O}_2}}}{y_{\text{CO}_2}^{\nu_{\text{CO}_2}}} \right) \left(\frac{2}{p_0} \right)^{\nu_{\text{CO}} + \nu_{\text{O}_2} - \nu_{\text{CO}_2}} \right] = \ln \left[\left(\frac{y_{\text{CO}}^1 y_{\text{O}_2}^{0.5}}{y_{\text{CO}_2}^1} \right) (2)^{1.5 - 1} \right] = \ln \left[\frac{\left(\frac{1 - a}{1 + \frac{4 - a}{2}} \right)^1 \left(\frac{\frac{4 - a}{2}}{1 + \frac{4 - a}{2}} \right)^{0.5}}{\left(\frac{a}{1 + \frac{4 - a}{2}} \right)^1} \times (2)^{0.5} \right];$$

$$\ln K_p = \ln \left[\left(\frac{1 - a}{1 + \frac{4 - a}{2}} \right) \left(\frac{1 + \frac{4 - a}{2}}{a} \right) \left(\frac{\frac{4 - a}{2}}{1 + \frac{4 - a}{2}} \right)^{0.5} \times (2)^{0.5} \right]; \quad \Rightarrow -6.635 = \ln \left[\left(\frac{1 - a}{a} \right) \left(\frac{4 - a}{6 - a} \right)^{0.5} \times (2)^{0.5} \right];$$

$$\begin{aligned} \Rightarrow e^{-6.635} &= \left[\left(\frac{1-a}{a} \right) \left(\frac{4-a}{6-a} \right)^{0.5} \times (2)^{0.5} \right]; \quad \Rightarrow 0.0013135787 = \left[\left(\frac{1-a}{a} \right) \left(\frac{4-a}{6-a} \right)^{0.5} \times (2)^{0.5} \right]; \\ \Rightarrow 1.725489 \times 10^{-6} &= \left[\left(\frac{1-a}{a} \right)^2 \left(\frac{4-a}{6-a} \right) (2) \right]; \quad \Rightarrow 1.725489 \times 10^{-6} = \left[\left(\frac{1-2a+a^2}{a^2} \right) \left(\frac{4-a}{6-a} \right) (2) \right]; \\ \Rightarrow 8.627445599 \times 10^{-7} &= \left[\frac{4-9a+6a^2-a^3}{6a^2-a^3} \right]; \\ \Rightarrow 5.176467359 \times 10^{-6} a^2 - 8.627445599 \times 10^{-7} a^3 &= 4-9a+6a^2-a^3; \\ \Rightarrow 0 &= 4-9a+5.999995a^2-0.9999991a^3; \quad \Rightarrow a = 0.998832 \end{aligned}$$

$$(a) \text{ O}_2 : \frac{4-a}{2} = \frac{4-0.998832}{2} = \mathbf{1.50058 \text{ kmol}}$$

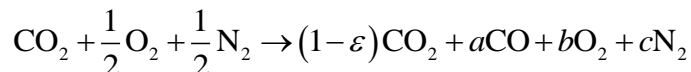
$$(b) \text{ CO}_2 : a = \mathbf{0.998832 \text{ kmol}}$$

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14-3-28 [BBF] A mixture of 1 kmol of CO₂, 1/2 kmol of O₂ and 1/2 kmol of N₂ is heated to 2900 K at a pressure of 1 atm. Determine the equilibrium composition of (a) CO₂, (b) O₂ assuming the mixture consists of CO₂, CO, O₂ and N₂.

SOLUTION

Molar Analysis:



$$\text{C: } 1 = (1-\varepsilon) + a; \quad \Rightarrow a = \varepsilon$$

$$\text{O: } 3 = 2(1-\varepsilon) + a + 2b; \quad \Rightarrow b = \frac{1+\varepsilon}{2}$$

$$\text{N: } 1 = 2c; \quad \Rightarrow c = \frac{1}{2}$$

Therefore:

$$(1-\varepsilon) + a + b + c = 1 - \varepsilon + \varepsilon + \frac{1+\varepsilon}{2} + \frac{1}{2} = \frac{4+\varepsilon}{2}$$

$$y_{\text{CO}_2} = \frac{(1-\varepsilon)}{4+\varepsilon} = \frac{2(1-\varepsilon)}{4+\varepsilon}; \quad y_{\text{CO}} = \frac{a}{4+\varepsilon} = \frac{2\varepsilon}{4+\varepsilon}; \quad y_{\text{O}_2} = \frac{b}{4+\varepsilon} = \frac{1+\varepsilon}{4+\varepsilon}; \quad y_{\text{N}_2} = \frac{c}{4+\varepsilon} = \frac{1}{4+\varepsilon}$$

For $\text{CO}_2 \rightleftharpoons \text{CO} + \frac{1}{2}\text{O}_2$ from Table G-3 at 2900 K, $\ln K_p \approx -1.5025$ and $p = 1$ atm

$$\ln K_p = \ln \left[\left(\frac{y_{\text{CO}}^{\nu_{\text{CO}}} y_{\text{O}_2}^{\nu_{\text{O}_2}}}{y_{\text{CO}_2}^{\nu_{\text{CO}_2}}} \right) \left(\frac{p}{p_0} \right)^{\nu_{\text{CO}} + \nu_{\text{O}_2} - \nu_{\text{CO}_2}} \right] = \ln \left[\left(\frac{y_{\text{CO}}^1 y_{\text{O}_2}^{0.5}}{y_{\text{CO}_2}^1} \right) (1)^{1.5-1} \right] = \ln \left[\frac{\left(\frac{2\varepsilon}{4+\varepsilon} \right)^1 \left(\frac{1+\varepsilon}{4+\varepsilon} \right)^{0.5}}{\left[\frac{2(1-\varepsilon)}{4+\varepsilon} \right]^1} \right];$$

$$\ln K_p = \ln \left[\left(\frac{\varepsilon}{1-\varepsilon} \right) \left(\frac{1+\varepsilon}{4+\varepsilon} \right)^{0.5} \right]; \quad \Rightarrow -1.5025 = \ln \left[\left(\frac{\varepsilon}{1-\varepsilon} \right) \left(\frac{1+\varepsilon}{4+\varepsilon} \right)^{0.5} \right];$$

$$\Rightarrow e^{-1.5025} = \left(\frac{\varepsilon}{1-\varepsilon} \right) \left(\frac{1+\varepsilon}{4+\varepsilon} \right)^{0.5}; \quad \Rightarrow 0.22257303 = \left(\frac{\varepsilon}{1-\varepsilon} \right) \left(\frac{1+\varepsilon}{4+\varepsilon} \right)^{0.5};$$

$$\Rightarrow 0.04953875 = \left(\frac{\varepsilon}{1-\varepsilon} \right)^2 \left(\frac{1+\varepsilon}{4+\varepsilon} \right); \quad \Rightarrow 0.04953875 = \frac{\varepsilon^3 + \varepsilon^2}{\varepsilon^3 + 2\varepsilon^2 - 7\varepsilon + 4};$$

$$\Rightarrow 0.04953875\varepsilon^3 + 0.0990775\varepsilon^2 - 0.34677125\varepsilon + 0.198155 = \varepsilon^3 + \varepsilon^2;$$

$$\Rightarrow 0.95046125\varepsilon^3 + 0.9009225\varepsilon^2 + 0.34677125\varepsilon - 0.198155 = 0;$$

$$\Rightarrow \varepsilon = 0.28877$$

(a) $\text{CO}_2 : (1 - \varepsilon) = (1 - 0.28877) = 0.71123 \text{ kmol}$

(b) $\text{O}_2 : \frac{1 + \varepsilon}{2} = \frac{1 + 0.28877}{2} = 0.6444 \text{ kmol}$

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14-3-29 [BBD] One kmol of carbon monoxide, CO, reacts with 1 kmol of oxygen, O₂, to form an equilibrium mixture of CO₂, CO and O₂ at 2800 K. Determine the equilibrium composition of CO₂ at (a) 1 atm, (b) 5 atm.

SOLUTION

Molar Analysis:



$$\text{C: } 1 = a + b; \quad \Rightarrow b = 1 - a$$

$$\text{O: } 3 = 2a + b + 2c; \quad \Rightarrow c = \frac{2-a}{2}$$

Therefore,

$$a + b + c = a + 1 - a + \frac{2-a}{2} = \frac{4-a}{2}$$

$$y_{\text{CO}_2} = \frac{2a}{4-a}; \quad y_{\text{CO}} = \frac{2-2a}{4-a}; \quad y_{\text{O}_2} = \frac{\frac{2-a}{2}}{\frac{4-a}{2}} = \frac{2-a}{4-a}$$

For $\text{CO}_2 \rightleftharpoons \text{CO} + \frac{1}{2}\text{O}_2$ from Table G-3 at 2800 K, $\ln K_p = -1.894$ and $p = 1$ atm

$$\ln K_p = \ln \left[\left(\frac{y_{\text{CO}}^{\nu_{\text{CO}}} y_{\text{O}_2}^{\nu_{\text{O}_2}}}{y_{\text{CO}_2}^{\nu_{\text{CO}_2}}} \right) \left(\frac{1}{p_0} \right)^{\nu_{\text{CO}} + \nu_{\text{O}_2} - \nu_{\text{CO}_2}} \right] = \ln \left[\left(\frac{y_{\text{CO}}^1 y_{\text{O}_2}^{0.5}}{y_{\text{CO}_2}^1} \right) (1)^{1.5-1} \right] = \ln \left[\frac{\left(\frac{2-2a}{4-a} \right) \left(\frac{2-a}{4-a} \right)^{0.5}}{\left(\frac{2a}{4-a} \right)^1} \right];$$

$$\ln K_p = \ln \left[\left(\frac{2-2a}{2a} \right) \left(\frac{2-a}{4-a} \right)^{0.5} \right]; \quad \Rightarrow -1.894 = \ln \left[\left(\frac{2-2a}{2a} \right) \left(\frac{2-a}{4-a} \right)^{0.5} \right];$$

$$\Rightarrow e^{-1.894} = \left[\left(\frac{2-2a}{2a} \right) \left(\frac{2-a}{4-a} \right)^{0.5} \right]; \quad \Rightarrow 0.1504687286 = \left[\left(\frac{2-2a}{2a} \right) \left(\frac{2-a}{4-a} \right)^{0.5} \right];$$

$$\Rightarrow 0.0226408383 = \left[\left(\frac{2-2a}{2a} \right)^2 \left(\frac{2-a}{4-a} \right) \right]; \quad \Rightarrow 0.0226408383 = \left[\frac{8-20a+16a^2-4a^3}{16a^2-4a^3} \right];$$

$$\Rightarrow 0.3622534124a^2 - 0.0905633531a^3 = 8 - 20a + 16a^2 - 4a^3;$$

$$\Rightarrow 0 = 8 - 20a + 15.63774659a^2 - 3.909436647a^3;$$

$$\Rightarrow a = 0.802643$$

$$\text{CO}_2 : a = \mathbf{0.8026 \text{ kmol}}$$

For $\text{CO}_2 \rightleftharpoons \text{CO} + \frac{1}{2} \text{O}_2$ from Table G-3 at 2800 K, $\ln K_p = -1.894$ and $p = 5 \text{ atm}$

$$\ln K_p = \ln \left[\left(\frac{y_{\text{CO}}^{\nu_{\text{CO}}} y_{\text{O}_2}^{\nu_{\text{O}_2}}}{y_{\text{CO}_2}^{\nu_{\text{CO}_2}}} \right) \left(\frac{5}{p_0} \right)^{\nu_{\text{CO}} + \nu_{\text{O}_2} - \nu_{\text{CO}_2}} \right] = \ln \left[\left(\frac{y_{\text{CO}}^1 y_{\text{O}_2}^{0.5}}{y_{\text{CO}_2}^1} \right) (5)^{1.5-1} \right] = \ln \left[\frac{\left(\frac{2-2a}{4-a} \right)^1 \left(\frac{2-a}{4-a} \right)^{0.5}}{\left(\frac{2a}{4-a} \right)^1} \times (5)^{0.5} \right];$$

$$\ln K_p = \ln \left[\left(\frac{2-2a}{2a} \right) \left(\frac{2-a}{4-a} \right)^{0.5} \times (5)^{0.5} \right]; \quad \Rightarrow -1.894 = \ln \left[\left(\frac{2-2a}{2a} \right) \left(\frac{2-a}{4-a} \right)^{0.5} \times (5)^{0.5} \right];$$

$$\Rightarrow e^{-1.894} = \left[\left(\frac{2-2a}{2a} \right) \left(\frac{2-a}{4-a} \right)^{0.5} \times (5)^{0.5} \right]; \quad \Rightarrow 0.1504687286 = \left[\left(\frac{2-2a}{2a} \right) \left(\frac{2-a}{4-a} \right)^{0.5} \times (5)^{0.5} \right];$$

$$\Rightarrow 0.0226408383 = \left[\left(\frac{2-2a}{2a} \right)^2 \left(\frac{2-a}{4-a} \right) \times (5) \right]; \quad \Rightarrow 0.0226408383 = \left[\frac{40 - 100a + 80a^2 - 20a^3}{16a^2 - 4a^3} \right];$$

$$\Rightarrow 0.3622534124a^2 - 0.0905633531a^3 = 40 - 100a + 80a^2 - 20a^3;$$

$$\Rightarrow 0 = 40 - 100a + 79.63774659a^2 - 19.909436647a^3;$$

$$\Rightarrow a = 0.898539$$

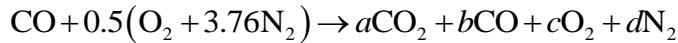
$$\text{CO}_2 : a = 0.8985 \text{ kmol}$$

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14-3-30 [BBM] One kmol of carbon monoxide (CO), reacts with theoretical amount of air to form an equilibrium mixture of CO₂, CO, O₂ and N₂ at 2200 K and 1 atm. Determine the equilibrium composition of (a) CO, (b) CO₂.

SOLUTION

Molar Analysis:



$$\text{C: } 1 = a + b; \quad \Rightarrow b = 1 - a$$

$$\text{O: } 2 = 2a + b + 2c; \quad \Rightarrow c = \frac{1-a}{2}$$

$$\text{N: } 3.76 = 2d; \quad \Rightarrow 1.88 = d$$

Therefore,

$$a + b + c + d = \frac{6.76 - a}{2}$$

$$y_{\text{CO}_2} = \frac{2a}{6.76 - a}; \quad y_{\text{CO}} = \frac{2 - 2a}{6.76 - a}; \quad y_{\text{O}_2} = \frac{\frac{1-a}{2}}{\frac{6.76 - a}{2}} = \frac{1-a}{6.76 - a}; \quad y_{\text{N}_2} = \frac{3.76}{6.76 - a}$$

For $\text{CO}_2 \rightleftharpoons \text{CO} + \frac{1}{2}\text{O}_2$ from Table G-3 at 2200 K, $\ln K_p = -5.120$ and $p = 1$ atm

$$\ln K_p = \ln \left[\left(\frac{y_{\text{CO}}^{\nu_{\text{CO}}} y_{\text{O}_2}^{\nu_{\text{O}_2}}}{y_{\text{CO}_2}^{\nu_{\text{CO}_2}}} \right) \left(\frac{1}{p_0} \right)^{\nu_{\text{CO}} + \nu_{\text{O}_2} - \nu_{\text{CO}_2}} \right] = \ln \left[\left(\frac{y_{\text{CO}}^1 y_{\text{O}_2}^{0.5}}{y_{\text{CO}_2}^1} \right) (1)^{1.5-1} \right] = \ln \left[\frac{\left(\frac{2-2a}{6.76-a} \right)^1 \left(\frac{1-a}{6.76-a} \right)^{0.5}}{\left(\frac{2a}{6.76-a} \right)^1} \right];$$

$$\ln K_p = \ln \left[\left(\frac{2-2a}{2a} \right) \left(\frac{1-a}{6.76-a} \right)^{0.5} \right]; \quad \Rightarrow -5.120 = \ln \left[\left(\frac{2-2a}{2a} \right) \left(\frac{1-a}{6.76-a} \right)^{0.5} \right];$$

$$\Rightarrow e^{-5.120} = \left[\left(\frac{2-2a}{2a} \right) \left(\frac{1-a}{6.76-a} \right)^{0.5} \right]; \quad \Rightarrow 0.0059760229 = \left[\left(\frac{2-2a}{2a} \right) \left(\frac{1-a}{6.76-a} \right)^{0.5} \right];$$

$$\Rightarrow 3.571284964 \times 10^{-5} = \left[\left(\frac{2-2a}{2a} \right)^2 \left(\frac{1-a}{6.76-a} \right) \right]; \quad \Rightarrow 3.571284964 \times 10^{-5} = \left[\frac{4 - 12a + 12a^2 - 4a^3}{27.04a^2 - 4a^3} \right];$$

$$\Rightarrow 9.656754543 \times 10^{-4} a^2 - 1.428513986 \times 10^{-4} a^3 = 4 - 12a + 12a^2 - 4a^3;$$

$$\Rightarrow 0 = 4 - 12a + 11.99903432a^2 - 3.999857149a^3;$$

$$\Rightarrow a = 0.943045$$

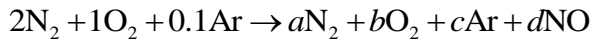
(a) CO: $1 - a = 1 - 0.943045 = 0.057$ kmol

(b) CO₂: $a = 0.943$ kmol

14-3-31 [BSR] A mixture of 2 kmol of N_2 , 1 kmol of O_2 and 0.1 kmol of Ar is heated to 2500 K at a constant pressure of 10 atm. Assuming the equilibrium mixture consists of N_2 , O_2 , Ar and NO, determine the equilibrium composition of (a) O_2 , (b) N_2 (in kmols).

SOLUTION

Molar Analysis:



$$N: 4 = 2a + d; \quad d = 4 - 2a$$

$$O: 2 = 2b + d; \quad b = \frac{2-d}{2} = \frac{-2+2a}{2}$$

$$Ar: 0.1 = c$$

Therefore,

$$a + b + c + d = 3.1$$

$$y_{N_2} = \frac{a}{3.1}; \quad y_{O_2} = \frac{\left(\frac{-2+2a}{2}\right)}{3.1} = \frac{-2+2a}{6.2}; \quad y_{NO} = \frac{4-2a}{3.1}; \quad y_{Ar} = \frac{0.1}{3.1}$$

For $\frac{1}{2}N_2 + \frac{1}{2}O_2 \rightleftharpoons NO$ from Table G-3 at 2500 K, $\ln K_p = -2.845$ and $p = 10$ atm

$$\begin{aligned} \ln K_p &= \ln \left[\left(\frac{y_{NO}^{v_{NO}}}{y_{O_2}^{v_{O_2}} y_{N_2}^{v_{N_2}}} \right) \left(\frac{10}{p_0} \right)^{v_{NO} - v_{O_2} - v_{N_2}} \right] = \ln \left[\left(\frac{y_{NO}^1}{y_{O_2}^{0.5} y_{N_2}^{0.5}} \right) (10)^{1-1} \right] = \ln \left[\frac{\left(\frac{4-2a}{3.1} \right)^1}{\left(\frac{-2+2a}{6.2} \right)^{0.5} \left(\frac{a}{3.1} \right)^{0.5}} \times (10)^0 \right]; \\ \ln K_p &= \ln \left[\left(\frac{4-2a}{3.1} \right) \left(\frac{6.2}{-2+2a} \right)^{0.5} \left(\frac{3.1}{a} \right)^{0.5} \right]; \quad \Rightarrow -2.845 = \ln \left[\left(\frac{4-2a}{3.1} \right) \left(\frac{6.2}{-2+2a} \right)^{0.5} \left(\frac{3.1}{a} \right)^{0.5} \right]; \\ \Rightarrow e^{-2.845} &= \left[\left(\frac{4-2a}{3.1} \right) \left(\frac{6.2}{-2+2a} \right)^{0.5} \left(\frac{3.1}{a} \right)^{0.5} \right]; \quad \Rightarrow 0.0581342667 = \left[\left(\frac{4-2a}{3.1} \right) \left(\frac{6.2}{-2+2a} \right)^{0.5} \left(\frac{3.1}{a} \right)^{0.5} \right]; \\ \Rightarrow 0.003379593 &= \left[\left(\frac{4-2a}{3.1} \right)^2 \left(\frac{6.2}{-2+2a} \right) \left(\frac{3.1}{a} \right) \right]; \quad \Rightarrow 0.003379593 = \left[\frac{32-32a+8a^2}{-2a+2a^2} \right]; \\ \Rightarrow -0.0067591859a &+ 0.0067591859a^2 = 32 - 32a + 8a^2; \\ \Rightarrow 0 &= 32 - 31.99324081a + 7.993240814a^2; \\ \Rightarrow a &= 1.96012 \end{aligned}$$

(a) $\text{O}_2 : \frac{-2+2a}{2} = \frac{-2+2(1.96012)}{2} = 0.96012 \text{ kmol}$

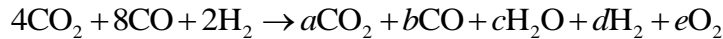
(b) $\text{N}_2 : a = 1.96012 \text{ kmol}$

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14-3-32 [BBJ] A chamber initially contains a gaseous mixture consisting of 4 kmol of CO₂, 8 kmol of CO and 2 kmol of H₂. Assume an equilibrium mixture formed consists of CO₂, CO, H₂O, H₂ and O₂ at 2600 K and 100 kPa, determine the equilibrium composition of (a) CO₂, (b) CO (in kmols).

SOLUTION

Molar Analysis:



$$\text{C: } 12 = a + b; \quad \Rightarrow b = 12 - a$$

$$\text{O: } 16 = 2a + b + c + 2e; \quad 4 = a + c + 2e$$

$$\text{H: } 4 = 2c + 2d; \quad \Rightarrow d = 2 - c$$

Therefore,

$$a + b + c + d + e = 14 + e$$

$$y_{\text{CO}_2} = \frac{a}{14+e}; \quad y_{\text{CO}} = \frac{b}{14+e} = \frac{12-a}{14+e}; \quad y_{\text{H}_2\text{O}} = \frac{c}{14+e}; \quad y_{\text{H}_2} = \frac{d}{14+e} = \frac{2-c}{14+e}; \quad y_{\text{O}_2} = \frac{e}{14+e}$$

For $\text{CO}_2 + \text{H}_2 \rightleftharpoons \text{CO} + \text{H}_2\text{O}$ from Table G-3 at 2600 K, $\ln K_p = 1.847$ and $p = 100$ kPa

$$\ln K_p = \ln \left[\left(\frac{y_{\text{CO}}^{\nu_{\text{CO}}} y_{\text{H}_2\text{O}}^{\nu_{\text{H}_2\text{O}}}}{y_{\text{CO}_2}^{\nu_{\text{CO}_2}} y_{\text{H}_2}^{\nu_{\text{H}_2}}} \right) \left(\frac{p}{p_0} \right)^{\nu_{\text{CO}} + \nu_{\text{H}_2\text{O}} - \nu_{\text{CO}_2} - \nu_{\text{H}_2}} \right] = \ln \left[\left(\frac{y_{\text{CO}}^1 y_{\text{H}_2\text{O}}^1}{y_{\text{CO}_2}^1 y_{\text{H}_2}^1} \right) (1)^{2-2} \right] = \ln \left[\frac{\left(\frac{12-a}{14+e} \right)^1 \left(\frac{c}{14+e} \right)^1}{\left(\frac{a}{14+e} \right)^1 \left(\frac{2-c}{14+e} \right)^1} \right];$$

$$\ln K_p = \ln \left[\left(\frac{14+e}{2-c} \right)^1 \left(\frac{14+e}{a} \right)^1 \left(\frac{12-a}{14+e} \right)^1 \left(\frac{c}{14+e} \right)^1 \right]; \quad \Rightarrow 1.847 = \ln \left[\frac{(12-a)c}{(2-c)a} \right];$$

$$\Rightarrow e^{1.847} = \left[\frac{12c - ac}{2a - ac} \right]; \quad \Rightarrow 6.340768655 = \left[\frac{12c - ac}{2a - ac} \right];$$

$$\Rightarrow 12.68153731a - 6.340768655ac = 12c - ac; \quad \Rightarrow 12.68153731a - 5.340768655ac = 12c;$$

$$\Rightarrow a(12.68153731 - 5.340768655c) = 12c;$$

$$\Rightarrow a = \frac{12c}{(12.68153731 - 5.340768655c)}$$

For $\text{CO}_2 \rightleftharpoons \text{CO} + \frac{1}{2}\text{O}_2$ from Table G-3 at 2600 K, $\ln K_p = -2.801$ and $p = 100$ kPa

$$\ln K_p = \ln \left[\left(\frac{y_{\text{CO}}^{v_{\text{CO}}} y_{\text{O}_2}^{v_{\text{O}_2}}}{y_{\text{CO}_2}^{v_{\text{CO}_2}}} \right) \left(\frac{p}{p_0} \right)^{v_{\text{CO}} + v_{\text{O}_2} - v_{\text{CO}_2}} \right] = \ln \left[\left(\frac{y_{\text{CO}}^1 y_{\text{O}_2}^{0.5}}{y_{\text{CO}_2}^1} \right) (1)^{1.5-1} \right] = \ln \left[\frac{\left(\frac{12-a}{14+e} \right)^1 \left(\frac{e}{14+e} \right)^{0.5}}{\left(\frac{a}{14+e} \right)^1} \right];$$

$$\ln K_p = \ln \left[\left(\frac{14+e}{a} \right)^1 \left(\frac{12-a}{14+e} \right)^1 \left(\frac{e}{14+e} \right)^{0.5} \right]; \Rightarrow -2.801 = \ln \left[\left(\frac{12-a}{a} \right)^1 \left(\frac{e}{14+e} \right)^{0.5} \right];$$

$$\Rightarrow e^{-2.801} = \left[\left(\frac{12-a}{a} \right)^1 \left(\frac{e}{14+e} \right)^{0.5} \right]; \Rightarrow 0.060749283 = \left[\left(\frac{12-a}{a} \right)^1 \left(\frac{e}{14+e} \right)^{0.5} \right];$$

$$\Rightarrow 0.0036904754 = \left[\left(\frac{12-a}{a} \right)^2 \left(\frac{e}{14+e} \right)^1 \right]; \Rightarrow 0.0036904754 = \left[\frac{144e - 24ae + a^2e}{14a^2 + a^2e} \right];$$

$$\Rightarrow 0.0516666553a^2 + 0.0036904754a^2e = 144e - 24ae + a^2e;$$

$$\Rightarrow 0.0516666553a^2 - 0.9963095246a^2e + 24ae - 144e = 0;$$

There are now three systems of equations and three variables to solve for.

$$(1) \quad 0.0516666553a^2 - 0.9963095246a^2e + 24ae - 144e = 0$$

$$(2) \quad a = \frac{12c}{(12.68153731 - 5.340768655c)}$$

$$(3) \quad 4 = a + c + 2e$$

Combining equations 2 and 3 together:

$$a = \frac{12(4 - a - 2e)}{(12.68153731 - 5.340768655(4 - a - 2e))} = \frac{48 - 12a - 24e}{-8.68153731 + 5.340768655a + 10.68153731e};$$

$$\Rightarrow -8.68153731a + 5.340768655a^2 + 10.68153731ea = 48 - 12a - 24e;$$

$$\Rightarrow 3.31846269a + 5.340768655a^2 - 48 = -24e - 10.68153731ea;$$

$$\Rightarrow 3.31846269a + 5.340768655a^2 - 48 = (-24 - 10.68153731a)e;$$

$$\Rightarrow e = \frac{3.31846269a + 5.340768655a^2 - 48}{-24 - 10.68153731a}$$

This can now be plugged into equation 1 to solve for a :

$$0.0516666553a^2 - 0.9963095246a^2e + 24ae - 144e = 0;$$

$$\begin{aligned}
&\Rightarrow 0.05a^2 - 0.996a^2 \left(\frac{3.3a + 5.3a^2 - 48}{-24 - 10.68a} \right) + 24a \left(\frac{3.3a + 5.3a^2 - 48}{-24 - 10.68a} \right) - 144 \left(\frac{3.3a + 5.3a^2 - 48}{-24 - 10.68a} \right) = 0; \\
&\Rightarrow 0.05a^2(-24 - 10.7a) - 0.996a^2(3a + 5a^2 - 48) + 24a(3a + 5a^2 - 48) - 144(3a + 5a^2 - 48) = 0; \\
&\Rightarrow -1.2a^2 - 0.6a^3 - 3.3a^3 - 5.3a^4 + 47.8a^2 + 79.6a^2 + 128.2a^3 - 1152a - 477.9a - 769.1a^2 + 6912 = 0; \\
&\Rightarrow -5.32105868a^4 + 124.3203524a^3 - 642.8447243a^2 - 1629.858627a + 6912 = 0; \\
&\Rightarrow a = 2.69617
\end{aligned}$$

(a) $\text{CO}_2 : a = 2.69617 \text{ kmol}$

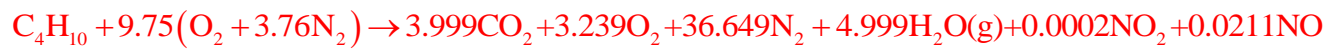
(b) $\text{CO} : b = 12 - a = 12 - 2.69617 = 9.30383 \text{ kmol}$

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14-3-33 [BBW] Butane (C_4H_{10}) burns inside a vessel with 50% excess air to form an equilibrium mixture at 1400 K and 1 MPa. The equilibrium mixture is composed of CO_2 , O_2 , N_2 , $H_2O(g)$, NO_2 , and NO . Determine the balanced reaction equation, using the IGE open-steady equilibrium TESTcalc.

SOLUTION

Using the IGE TESTcalc, the following equation is obtained:



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14-3-34 [BSO] Methane (CH_4) reacts with 125% of theoretical air inside a chamber to form an equilibrium mixture consisting of CO_2 , CO , $\text{H}_2\text{O}(\text{g})$, H_2 , and N_2 at 1200 K, 100 kPa. Determine the equilibrium composition of (a) CO_2 , (b) H_2O (in kmols) using the IGE open-steady equilibrium TESTcalc.

SOLUTION

Using the IGE TESTcalc, the following equation is obtained:

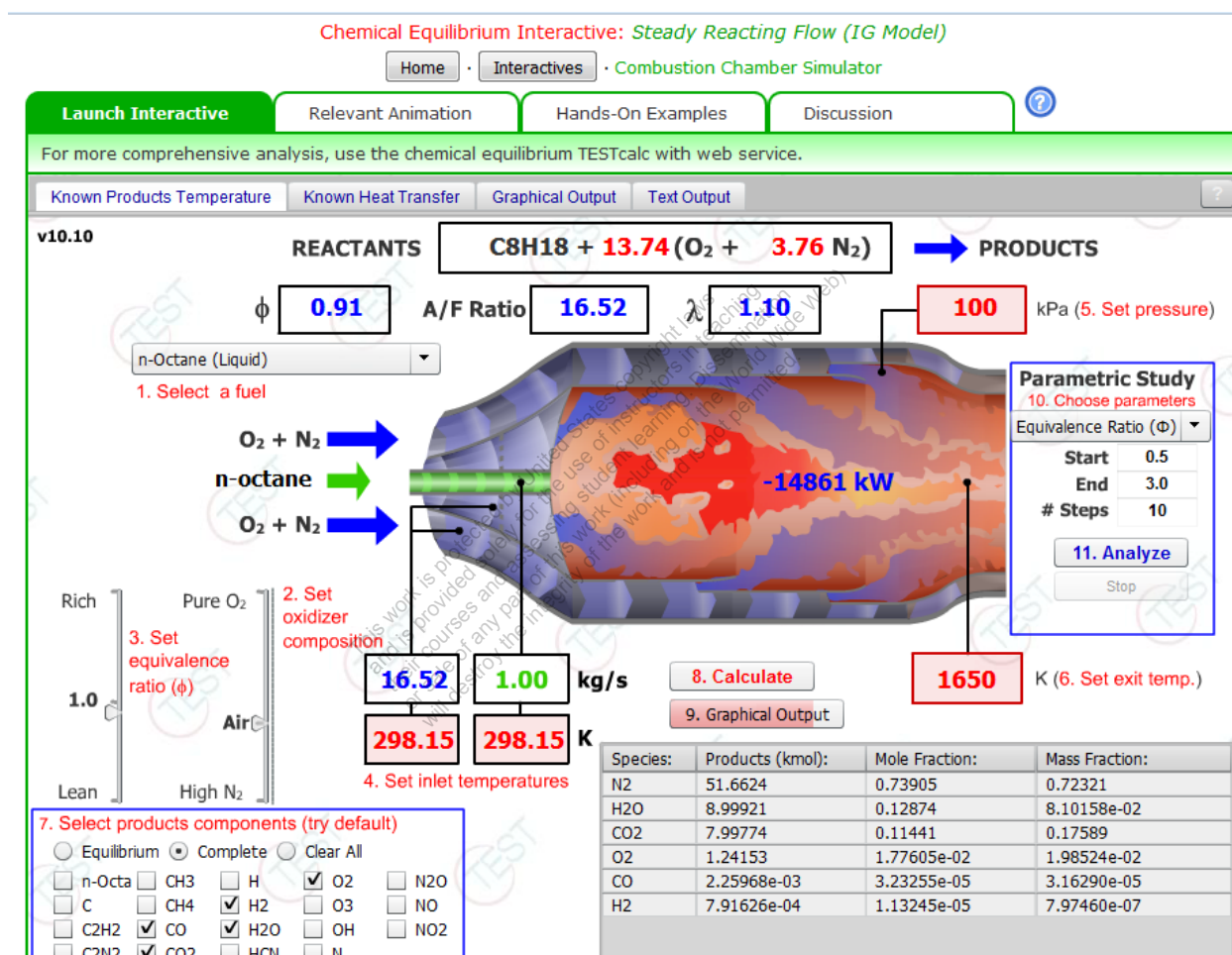


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14-3-35 [BSB] Octane (C_8H_{18}) reacts with 110% of theoretical air inside a chamber to form an equilibrium mixture consists of CO_2 , CO , $H_2O(g)$, H_2 , O_2 , and N_2 at 1650 K, 100 kPa. Determine the composition of the equilibrium mixture using the equilibrium combustion interactive.

SOLUTION

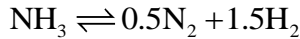
Start the equilibrium interactive. Adjust the air fuel ratio with the slide bar so that lambda becomes 1.1. Select the products species, change the exit temperature to 1650 K and click Calculate. The following output is generated by the interactive:



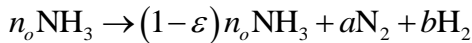
14-3-36 [BSS] Starting with n_0 kmol of NH_3 , which dissociates according to $\text{NH}_3 \leftrightarrow (1/2)\text{N}_2 + (3/2)\text{H}_2$, evaluate an expression for K in terms of the degree of dissociation ε and pressure p .

SOLUTION

The theoretical reaction is given as:



Molar Analysis:



$$\text{N: } n_0 = (1-\varepsilon)n_0 + 2a; \quad \Rightarrow a = \frac{n_0\varepsilon}{2}$$

$$\text{H: } 3n_0 = 3(1-\varepsilon)n_0 + 2b; \quad \Rightarrow b = \frac{3n_0\varepsilon}{2}$$

Therefore,

$$(1-\varepsilon)n_0 + a + b = (1-\varepsilon)n_0 + \frac{n_0\varepsilon}{2} + \frac{3n_0\varepsilon}{2};$$

$$\Rightarrow \frac{2(1-\varepsilon)n_0 + n_0\varepsilon + 3n_0\varepsilon}{2} = \frac{2n_0 + 2n_0\varepsilon}{2} = n_0 + n_0\varepsilon = (1+\varepsilon)n_0$$

$$y_{\text{NH}_3} = \frac{(1-\varepsilon)n_0}{(1+\varepsilon)n_0} = \frac{1-\varepsilon}{1+\varepsilon}; \quad y_{\text{N}_2} = \frac{a}{(1+\varepsilon)n_0} = \frac{n_0\varepsilon}{2(1+\varepsilon)n_0} = \frac{0.5\varepsilon}{1+\varepsilon}; \quad y_{\text{CO}_2} = \frac{b}{(1+\varepsilon)n_0} = \frac{3n_0\varepsilon}{2(1+\varepsilon)n_0} = \frac{1.5\varepsilon}{1+\varepsilon}$$

$$K = \left(\frac{y_{\text{N}_2}^{v_{\text{N}_2}} y_{\text{H}_2}^{v_{\text{H}_2}}}{y_{\text{NH}_3}^{v_{\text{NH}_3}}} \right) \left(\frac{p}{p_0} \right)^{v_{\text{N}_2} + v_{\text{H}_2} - v_{\text{NH}_3}} = \left(\frac{y_{\text{N}_2}^{0.5} y_{\text{H}_2}^{1.5}}{y_{\text{NH}_3}^1} \right) \left(\frac{p}{p_0} \right)^{2-1};$$

$$K = \frac{\left(\frac{0.5\varepsilon}{1+\varepsilon} \right)^{0.5} \left(\frac{1.5\varepsilon}{1+\varepsilon} \right)^{1.5}}{\left(\frac{1-\varepsilon}{1+\varepsilon} \right)^1} \times \left(\frac{p}{p_0} \right) = \left(\frac{0.5\varepsilon}{1+\varepsilon} \right)^{0.5} \left(\frac{1.5\varepsilon}{1+\varepsilon} \right)^{1.5} \left(\frac{1+\varepsilon}{1-\varepsilon} \right)^1 \left(\frac{p}{p_0} \right);$$

$$K^2 = \left(\frac{0.5\varepsilon}{1+\varepsilon} \right)^1 \left(\frac{1.5\varepsilon}{1+\varepsilon} \right)^3 \left(\frac{1+\varepsilon}{1-\varepsilon} \right)^2 \left(\frac{p}{p_0} \right)^2 = \frac{(0.5\varepsilon)(1.5^3\varepsilon^3)}{(1+\varepsilon)^2(1-\varepsilon)^2} \left(\frac{p}{p_0} \right)^2;$$

$$K^2 = \frac{1.6875\varepsilon^4}{(1+\varepsilon)^2(1-\varepsilon)^2} \left(\frac{p}{p_0} \right)^2;$$

$$K = \frac{1.299\varepsilon^2}{(1+\varepsilon)(1-\varepsilon)} \left(\frac{p}{p_0} \right) = \frac{1.299\varepsilon^2}{1-\varepsilon^2} \left(\frac{p}{p_0} \right)$$

14-3-37 [BSA] Determine the mole fraction of sodium that ionizes according to the reaction $\text{Na} \leftrightarrow \text{Na}^+ + \text{e}^-$ at 2300 K and 0.5 atm (use $K = 0.688$ for this reaction).

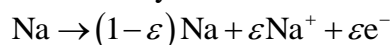
SOLUTION

Given: $T = 2300 \text{ K}$; $p = 0.5 \text{ atm}$;

$K = 0.688$;



Molar Analysis:



Therefore,

$$1 - \varepsilon + \varepsilon + \varepsilon = 1 + \varepsilon$$

$$y_{\text{Na}} = \frac{1 - \varepsilon}{1 + \varepsilon}; \quad y_{\text{Na}^+} = \frac{\varepsilon}{1 + \varepsilon}; \quad y_{\text{e}^-} = \frac{\varepsilon}{1 + \varepsilon}$$

$$K = \left(\frac{y_p^{v_p}}{y_r^{v_r}} \right) \left(\frac{p}{p_0} \right)^{\sum v_p - \sum v_r} = \left(\frac{y_{\text{Na}^+}^{v_{\text{Na}^+}} y_{\text{e}^-}^{v_{\text{e}^-}}}{y_{\text{Na}}^{v_{\text{Na}}}} \right) \left(\frac{p}{p_0} \right)^{v_{\text{Na}^+} + v_{\text{e}^-} - v_{\text{Na}}} = \left(\frac{y_{\text{Na}^+}^1 y_{\text{e}^-}^1}{y_{\text{Na}}^1} \right) \left(\frac{p}{p_0} \right)^{2-1};$$

$$K = \frac{\left(\frac{\varepsilon}{1 + \varepsilon} \right) \left(\frac{\varepsilon}{1 + \varepsilon} \right)}{\left(\frac{1 - \varepsilon}{1 + \varepsilon} \right)} \times \left(\frac{0.5}{1} \right) = \frac{0.5\varepsilon^2}{(1 + \varepsilon)(1 - \varepsilon)} = \frac{0.5\varepsilon^2}{1 - \varepsilon^2};$$

$$\Rightarrow 1.376 = \frac{\varepsilon^2}{1 - \varepsilon^2};$$

$$\Rightarrow 2.376\varepsilon^2 - 1.376 = 0;$$

$$\Rightarrow \varepsilon = 0.7610$$

14-3-38 [BSH] Determine the percent ionization of cesium that ionizes according to the reaction $\text{Ce} \leftrightarrow \text{Ce}^+ + \text{e}^-$ at 2000 K and 1 atm (use $K = 15.63$ for this reaction).

SOLUTION

Given: $T = 2000 \text{ K}$; $p = 1 \text{ atm}$;

$K = 15.63$;



Molar Analysis:



Therefore

$$1 - \varepsilon + \varepsilon + \varepsilon = 1 + \varepsilon$$

$$y_{\text{Ce}} = \frac{1 - \varepsilon}{1 + \varepsilon}; \quad y_{\text{Ce}^+} = \frac{\varepsilon}{1 + \varepsilon}; \quad y_{\text{e}^-} = \frac{\varepsilon}{1 + \varepsilon}$$

$$K = \left(\frac{y_p^{\nu_p}}{y_r^{\nu_r}} \right) \left(\frac{p}{p_0} \right)^{\sum \nu_p - \sum \nu_r} = \left(\frac{y_{\text{Ce}^+}^{\nu_{\text{Ce}^+}} y_{\text{e}^-}^{\nu_{\text{e}^-}}}{y_{\text{Ce}}^{\nu_{\text{Ce}}}} \right) \left(\frac{p}{p_0} \right)^{\nu_{\text{Ce}^+} + \nu_{\text{e}^-} - \nu_{\text{Ce}}} = \left(\frac{y_{\text{Ce}^+}^1 y_{\text{e}^-}^1}{y_{\text{Ce}}^1} \right) \left(\frac{p}{p_0} \right)^{2-1};$$

$$K = \frac{\left(\frac{\varepsilon}{1 + \varepsilon} \right) \left(\frac{\varepsilon}{1 + \varepsilon} \right)}{\left(\frac{1 - \varepsilon}{1 + \varepsilon} \right)} \times \left(\frac{1}{1} \right) = \frac{\varepsilon^2}{(1 + \varepsilon)(1 - \varepsilon)} = \frac{\varepsilon^2}{1 - \varepsilon^2};$$

$$\Rightarrow 15.63 = \frac{\varepsilon^2}{1 - \varepsilon^2};$$

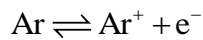
$$\Rightarrow 16.63\varepsilon^2 - 15.63 = 0;$$

$$\Rightarrow x = 0.9694 = 96.94\%$$

14-3-39 [BSN] Determine (a) the pressure if the ionization of Ar is 80% complete according to the reaction $\text{Ar} \leftrightarrow \text{Ar}^+ + \text{e}^-$ at 10,000 K (use $K = 4.2 \times 10^{-4}$ for this reaction). (b) What-if Scenario: What would the pressure be if the ionization of Ar is 50% complete instead?

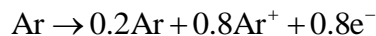
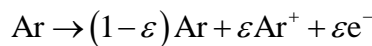
SOLUTION

Given: $T = 10,000 \text{ K}$



$$\varepsilon = 0.8$$

Molar Analysis:



Therefore,

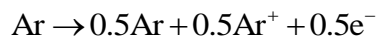
$$0.2 + 0.8 + 0.8 = 1.8$$

$$y_{\text{Ar}} = \frac{0.2}{1.8}; \quad y_{\text{Ar}^+} = \frac{0.8}{1.8}; \quad y_{\text{e}^-} = \frac{0.8}{1.8}$$

$$K = \left(\frac{y_p^{\nu_p}}{y_r^{\nu_r}} \right) \left(\frac{p}{p_0} \right)^{\sum \nu_p - \sum \nu_r} = \left(\frac{y_{\text{Ar}^+}^{\nu_{\text{Ar}^+}} y_{\text{e}^-}^{\nu_{\text{e}^-}}}{y_{\text{Ar}}^{\nu_{\text{Ar}}}} \right) \left(\frac{p}{p_0} \right)^{\nu_{\text{Ar}^+} + \nu_{\text{e}^-} - \nu_{\text{Ar}}} = \left(\frac{y_{\text{Ar}^+}^1 y_{\text{e}^-}^1}{y_{\text{Ar}}^1} \right) \left(\frac{p}{p_0} \right)^{2-1};$$

$$4.2 \times 10^{-4} = \frac{\left(\frac{0.2}{1.8} \right) \left(\frac{0.8}{1.8} \right)}{\left(\frac{0.8}{1.8} \right)} \left(\frac{p}{p_0} \right) = 0.11111111 \left(\frac{p}{p_0} \right);$$

$$\Rightarrow p = 0.00378 \text{ atm}$$



Therefore,

$$0.5 + 0.5 + 0.5 = 1.5$$

$$y_{\text{Ar}} = \frac{0.5}{1.5}; \quad y_{\text{Ar}^+} = \frac{0.5}{1.5}; \quad y_{\text{e}^-} = \frac{0.5}{1.5}$$

$$K = \left(\frac{y_p^{V_p}}{y_r^{V_r}} \right) \left(\frac{p}{p_0} \right)^{\sum V_p - \sum V_r} = \left(\frac{y_{Ar^+}^{V_{Ar^+}} y_{e^-}^{V_{e^-}}}{y_{Ar}^{V_{Ar}}} \right) \left(\frac{p}{p_0} \right)^{V_{Ar^+} + V_{e^-} - V_{Ar}} = \left(\frac{y_{Ar^+}^1 y_{e^-}^1}{y_{Ar}^1} \right) \left(\frac{p}{p_0} \right)^{2-1};$$

$$4.2 \times 10^{-4} = \frac{\left(\frac{0.5}{1.5} \right) \left(\frac{0.5}{1.5} \right)}{\left(\frac{0.5}{1.5} \right)} \left(\frac{p}{p_0} \right) = 0.333333 \left(\frac{p}{p_0} \right);$$

$$\Rightarrow p = \mathbf{0.00126 \text{ atm}}$$

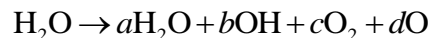
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14-3-40 [BSE] One kmol of H_2O is heated to 3000 K at a pressure of 1 atm. Determine the equilibrium composition of H_2O (in kmols) assuming that only H_2O , OH , O_2 and O are present.

SOLUTION

$$T = 3000 \text{ K}; p = 1 \text{ atm}$$

Molar analysis:



Looking at the molar analysis, if any of the H_2O were to dissociate, the water would only be able to dissociate into OH which would cause the reaction to be unbalanced due to a floating hydrogen atom. Therefore,

$$\text{H}_2\text{O} = 1 \text{ kmol}$$

TEST Solution:

TEST-Specific, Closed Process, Chem. Equilibrium Daemon: IG model

$$a = 0.9999978; b = 0.0000023; c = 7.565 \times 10^{-21}; d = 9.79 \times 10^{-12}$$

$$\text{H}_2\text{O} = 0.9999978; \text{OH} = 0.0000022; \text{O}_2 = 1.3434 \times 10^{-20}; \text{O} = 8.6928 \times 10^{-21}$$

Check the result from TEST in Balance Equation

$$\text{H}: 2 = 2a + b \rightarrow 2(0.9999978) + 0.0000023 = 1.9999979(1.05 \times 10^{-4})$$

$$\text{O}: 1 = a + b + 2c + d \rightarrow 0.9999978 + 0.0000023 + 7.565 \times 10^{-21} + 9.79 \times 10^{-12} = 1.0000001$$

$$\text{H}_2\text{O} = 0.9999978 \text{ kmol}$$

14-3-41 [BSI] A mixture of 2 kmol of CO₂ and 1 kmol of O₂ is heated to 3200 K at a pressure of 5 atm. Determine the equilibrium composition of (a) CO, (b) CO₂ (in kmols) using the IGE open-steady equilibrium TESTcalc assuming that only CO₂, CO, O₂ and O are present.

SOLUTION

Using the IGE TESTcalc, the following equation is obtained:

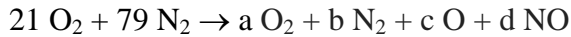


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14-3-42 [BSG] Air (21% O₂, 79% N₂) is heated to 2800 K at a pressure of 1 atm. Determine the equilibrium composition, assuming that only O₂, N₂, O and NO are present. Can the presence of NO in the equilibrium mixture be neglected?

SOLUTION

Molar Analysis:



$$\text{O: } 42 = 2a + c + d; \quad \Rightarrow d = 42 - 2a - c$$

$$\text{N: } 158 = 2b + d; \quad \Rightarrow b = 79 - 0.5d; \quad \Rightarrow b = 79 - 21 + a + 0.5c; \quad \Rightarrow b = 58 + a + 0.5c$$

$$\text{Total: } a + b + c + d = a + 58 + a + 0.5c + c + 42 - 2a - c = 100 + 0.5c$$

$$y_{\text{O}_2} = \frac{a}{100 + 0.5c}; \quad y_{\text{N}_2} = \frac{b}{100 + 0.5c} = \frac{58 + a + 0.5c}{100 + 0.5c};$$

$$y_{\text{O}} = \frac{c}{100 + 0.5c}; \quad y_{\text{NO}} = \frac{d}{100 + 0.5c} = \frac{42 - 2a - c}{100 + 0.5c}$$

Now we use:

$$\text{O}_2 \rightleftharpoons 2\text{O} \text{ gives us } \ln K_{p@2800\text{K}} = -5.826$$

$$\frac{1}{2}\text{N}_2 + \frac{1}{2}\text{O}_2 \rightleftharpoons \text{NO} \text{ gives us } \ln K_{p@2800\text{K}} = -2.372$$

$$K_p = \frac{y_{\text{O}}^2}{y_{\text{O}_2}} \left(\frac{p}{p_0} \right)^{2-1} = [p = p_0] = \frac{y_{\text{O}}^2}{y_{\text{O}_2}} = \frac{\left(\frac{c}{\sum \nu_p} \right)^2}{\frac{a}{\sum \nu_p}} = \frac{c^2}{(21 - 0.5c - 0.5d)(100 + 0.5c)} = e^{-5.826} \Leftrightarrow$$

$$\Leftrightarrow f(c, d) = c^2 - e^{-5.826} (21 - 0.5c - 0.5d)(100 + 0.5c) = 0$$

$$K_p = \frac{y_{\text{NO}}}{\sqrt{y_{\text{N}_2}} \sqrt{y_{\text{O}_2}}} \left(\frac{p}{p_0} \right) = [p = p_0] = \frac{y_{\text{NO}}}{\sqrt{y_{\text{N}_2}} \sqrt{y_{\text{O}_2}}} = \frac{\frac{d}{\sum \nu_p}}{\frac{\sqrt{b} \sqrt{a}}{\sum \nu_p}} = \frac{d}{\sqrt{21 - 0.5c - 0.5d} \sqrt{79 - 0.5d}} = e^{-2.372} \Leftrightarrow$$

$$\Leftrightarrow g(c, d) = d - e^{-2.372} \sqrt{21 - 0.5c - 0.5d} \sqrt{79 - 0.5d} = 0$$

TEST calculations gives: $a \approx 18.08008$; $b \approx 77.23361$; $c \approx 2.30862$; $d \approx 3.53065$

Let us now see that the equations we have above satisfy that:

$$f(c, d) \approx -0.065$$

$$g(c, d) \approx 0.044$$

This is close enough to be true since K_p as well as a , b , c & d are not as exact as in TEST so it should be some discrepancy.

To find the equilibrium composition we must find the relative mole fraction:

$$y_{O_2} = \frac{a}{100 + 0.5c} \approx 0.17874; \quad y_{N_2} = \frac{b}{100 + 0.5c} \approx 0.76352; \quad y_O = \frac{c}{100 + 0.5c} \approx 0.02282;$$

$$y_{NO} = \frac{d}{100 + 0.5c} \approx 0.03490$$

If we don't assume we have any NO: $21 O_2 + 79 N_2 \rightarrow a O_2 + b N_2 + c O$

TEST gives us: $a \approx 19.79194$; $b \approx 78.99996$; $c \approx 2.41610$

The equilibrium composition is 17.9% O_2 , 76.4% N_2 + 2.3% O + 3.5 % NO

As the TEST calculations above shows NO can **not** be neglected as a product. N , N_2O , NO_2 & O_3 on the other hand can be neglected as products (*verified with a TEST calculation*)

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14-3-43 [BSL] The equilibrium constant for dissociation of N_2O_4 is 0.664 and 0.141 at 318 K and 298 K respectively. Calculate the average heat of reaction within this temperature range.

SOLUTION

Given:

$$T_1 = 318 \text{ K};$$

$$T_2 = 298 \text{ K};$$

$$K_1 = 0.664;$$

$$K_2 = 0.141;$$

$$\ln \frac{K_2}{K_1} = \frac{-\left(\Delta \bar{h}_r^\circ\right)}{\bar{R}} \left[\frac{1}{T_2} - \frac{1}{T_1} \right]; \quad \Rightarrow \Delta \bar{h}_r^\circ = \bar{R} \frac{\ln \frac{K_2}{K_1}}{\left(\frac{1}{T_1} - \frac{1}{T_2} \right)};$$

$$\Delta \bar{h}_r^\circ = 8.314 \frac{\ln \frac{0.141}{0.664}}{\left(\frac{1}{318} - \frac{1}{298} \right)};$$

$$\Rightarrow \Delta \bar{h}_r^\circ = 61,040 \frac{\text{kJ}}{\text{kmol}}$$

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14-3-44 [BSK] At an average temperature of 2000 K, the slope of the graph of $\log K$ against $1/T$ for the dissociation of water vapor (into hydrogen and oxygen) is found to be -13000. (a) Determine the heat of dissociation. (b) Is this an exothermic reaction?

SOLUTION

$$\ln \frac{K_2}{K_1} = -\frac{(\Delta \bar{h}_r^\circ)}{\bar{R}} \left[\frac{1}{T_2} - \frac{1}{T_1} \right];$$

$$\Rightarrow \frac{\ln \frac{K_2}{K_1}}{\frac{1}{T_2} - \frac{1}{T_1}} = -13000 = -\frac{(\Delta \bar{h}_r^\circ)}{\bar{R}};$$

$$\Rightarrow \Delta \bar{h}_r^\circ = 13000 \bar{R} = (13000)(8.314) = 108082 \frac{\text{kJ}}{\text{kmol}}$$

No, a positive heat of dissociation means the reaction is endothermic.

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14-3-45 [BSU] Potassium is ionized according to the equation $K \leftrightarrow K^+ + e^-$. The values of equilibrium constants at 3000 K and 3500 K are measured to be 8.33×10^{-6} and 1.33×10^{-4} respectively. Determine the average heat of reaction in MJ/kmol.

SOLUTION

Given:

$$T_1 = 3000 \text{ K};$$

$$T_2 = 3,500 \text{ K};$$

$$K_1 = 8.33 \times 10^{-6};$$

$$K_2 = 1.33 \times 10^{-4};$$

$$\ln \frac{K_2}{K_1} = \frac{-(\Delta \bar{h}_T^\circ)}{\bar{R}} \left[\frac{1}{T_2} - \frac{1}{T_1} \right]; \quad \Rightarrow \Delta \bar{h}_T^\circ = \bar{R} \frac{\ln \frac{K_2}{K_1}}{\left(\frac{1}{T_1} - \frac{1}{T_2} \right)};$$

$$\Delta \bar{h}_T^\circ = 8.314 \frac{\ln \frac{1.33 \times 10^{-4}}{8.33 \times 10^{-6}}}{\left(\frac{1}{3,000} - \frac{1}{3,500} \right)};$$

$$\Rightarrow \Delta \bar{h}_T^\circ = 483.71 \frac{\text{MJ}}{\text{kmol}}$$

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14-3-46 [BSZ] The equilibrium constant for the reaction $\text{SO}_3 \leftrightarrow \text{SO}_2 + \text{O}$ has the following values:

T	800 K	900 K	1000 K	1105 K
K	0.0319	0.153	0.540	1.59

Determine the average heat of dissociation using graphical method.

SOLUTION

$$\ln \frac{K_2}{K_1} = \frac{-(\Delta \bar{h}_T^\circ)}{R} \left[\frac{1}{T_2} - \frac{1}{T_1} \right]; \quad \Rightarrow \Delta \bar{h}_T^\circ = R \frac{\ln \frac{K_2}{K_1}}{\left(\frac{1}{T_1} - \frac{1}{T_2} \right)};$$

$$\Delta \bar{h}_{T,1 \rightarrow 2}^\circ = 8.314 \frac{\ln \left(\frac{0.153}{0.0319} \right)}{\left(\frac{1}{800} - \frac{1}{900} \right)} = 93.851 \frac{\text{MJ}}{\text{kmol}}$$

$$\Delta \bar{h}_{T,2 \rightarrow 3}^\circ = 8.314 \frac{\ln \left(\frac{0.540}{0.153} \right)}{\left(\frac{1}{900} - \frac{1}{1000} \right)} = 94.365 \frac{\text{MJ}}{\text{kmol}}$$

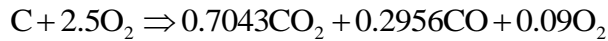
$$\Delta \bar{h}_{T,3 \rightarrow 4}^\circ = 8.314 \frac{\ln \left(\frac{1.59}{0.540} \right)}{\left(\frac{1}{1000} - \frac{1}{1105} \right)} = 94.487 \frac{\text{MJ}}{\text{kmol}}$$

$$\Delta \bar{h}_T^\circ = \frac{\Delta \bar{h}_{T,1 \rightarrow 2}^\circ + \Delta \bar{h}_{T,2 \rightarrow 3}^\circ + \Delta \bar{h}_{T,3 \rightarrow 4}^\circ}{3} = \frac{93.851 + 94.365 + 94.487}{3} = 94.234 \frac{\text{MJ}}{\text{kmol}}$$

14-3-47 [BVT] 1 kmol of Carbon at 25°C, 0.1 MPa reacts with 2.5 kmol of oxygen at 25°C, 0.1 MPa form an equilibrium mixture of CO₂, CO and O₂ at 3000 K, 0.1 MPa. Determine (a) the amount of CO₂ present in the products mixture and (b) heat transfer for the process.

SOLUTION

Using the IGE open-steady equilibrium TESTcalc, the following equilibrium reaction is found:



$$CO_2 = 0.7043 \text{ kmol}$$

The enthalpies for the products and the reactants are also found as

$$h_R = 7789.327 \frac{\text{kJ}}{\text{kg}}$$

$$h_P = -139.874 \frac{\text{kJ}}{\text{kg}}$$

The mass involved in the reaction,

$$m = m_C + m_{O_2} = n_C \bar{M}_C + n_{O_2} \bar{M}_{O_2} = (1)(12) + (2.5)(32) = 92 \text{ kg}$$

Therefore, the heat transfer in this process,

$$Q - \cancel{W_{\text{ext}}}^0 = m(h_P - h_R) = (92)(-139.874 - 7789.327) = -729486.49 \text{ kJ} = -729.486 \text{ MW}$$

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14-3-48 [BSY] For the reaction in the previous problem, 14-3-47 [BVT], plot how heat transfer varies with equivalence ratio varying from 0.1 to 1, all other parameters remaining unchanged.

SOLUTION

Keeping in mind that the equivalence ratio is the inverse of theoretical air $\phi = 1/\lambda$,

Parameter		Reactants			Products			Results			
lambda	phi	n_C	n_O2	n_N2	n_CO2	n_O2	n_N2	m	h_R	h_P	Q
unitless	unitless	[kmol]	[kmol]	[kmol]	[kmol]	[kmol]	[kmol]	[kg]	[kJ/kg]	[kJ/kg]	[MW]
10	0.1	1	10	37.6	1	9	37.6	1385.302	62.2	2980.07	4042.132
5	0.2	1	5	18.8	1	4	18.8	698.6567	123.33	2712.1	1808.662
3.333333	0.3	1	3.333333	12.53333	1	2.333333	12.53333	469.7748	183.41	2448.69	1064.171
2.5	0.4	1	2.5	9.4	1	1.5	9.4	355.3339	242.49	2189.73	691.9203
2	0.5	1	2	7.52	1	1	7.52	286.6693	300.57	1935.12	468.5753
1.666667	0.6	1	1.666667	6.266667	1	0.666667	6.266667	240.8929	357.68	1684.73	319.6769
1.428571	0.7	1	1.428571	5.371429	1	0.428571	5.371429	208.1955	413.86	1438.47	213.3192
1.25	0.8	1	1.25	4.7	1	0.25	4.7	183.6724	469.12	1196.23	133.5501
1.111111	0.9	1	1.111111	4.177778	1	0.111111	4.177778	164.5989	523.48	957.92	71.50836
1	1	1	1	3.76	1	0	3.76	149.3401	576.97	723.6233	21.90122

Heat Transfer per kmol of C vs Equivalence Ratio

