Solutions tot he examples of the theoretical questions at the 43rd IChO

Problem [1]

a)

Gas constant: R = 0.08205 atm·L·K^{-1}·mol^{-1}

$$n_{H_2} = \frac{\left(100\times10^{-3}\ L\cdot\min^{-1}\right)\times\left(1.0\ atm\right)}{\left(0.082\ atm\cdot L\cdot K^{-1}\cdot mol^{-1}\right)} = 4.1\times10^{-3}\ mol\ H_2\cdot\min^{-1}$$

$$\frac{\left(4.1\times10^{-3}\ mol\ H_2\cdot\min^{-1}\right)}{\left(92\ mol\ H_2\cdot\left(mol\ Ru\right)^{-1}\cdot\min^{-1}\right)} = 4.5\times10^{-5}\ mol\ Ru$$

$$\left(4.5\times10^{-5}\ mol\ Ru\right)\times\left(101.07\ g\cdot mol^{-1}\right) = 4.5\times10^{-3}\ g\ Ru = 4.5\ mg\ Ru$$

b)

$$\left(1.00\times10^{-1}\ L\right)\times\left(1.0\ mol\cdot L^{-1}\right) = 0.10\ mol\ NaBH_4$$

$$\left(0.10\ mol\ NaBH_4\right)\times 4\ mol\ H_2\cdot\left(mol\cdot NaBH_4\right)^{-1} = 0.40\ mol\ H_2\ \ to\ be\ released$$

$$\frac{\left(0.40\ mol\ H_2\right)}{\left(4.1\times10^{-3}\ mol\ H_2\cdot\min^{-1}\right)} = 98\ \min$$

c)

$$Rate = k\left[Ru\right] = \left(A\cdot e^{-E_a/RT}\right)\left[Ru\right]$$

$$\frac{\left(e^{-E_a/R\,298}\right)}{\left(e^{-E_a/RT}\right)} = \frac{1}{2}$$

$$-\frac{E_a}{R}\left(\frac{1}{298}-\frac{1}{T}\right) = \ln\left(\frac{1}{2}\right),\quad \frac{4.20\times10^4\ J\cdot mol^{-1}}{8.314\ J\cdot K^{-1}\cdot mol^{-1}}\left(\frac{1}{298}-\frac{1}{T}\right) = \ln\left(2\right)$$

$$T = 311\,K\ \ or\ \ T = 38\,°C$$

d)

$$Since\ \Delta G° = -nFE°$$

$$2\left(-2.37\times10^{5}\right)=-4\times96485\times E^{o}_{cell} \qquad E^{o}_{cell}=+1.23\,V$$

$$1.23\,V=E^{o}_{cathode}-\left(-0.83\,V\right) \qquad E^{o}_{cathode}=+0.40\,V$$

e)

$$\left(2.5\,A\right)\times\left(3.0\,h\right)\times\left(3600\,s\cdot h^{-1}\right)=27000\,C$$

$$n\left(O_2\right)=\left(27000\,C\right)\times\left(\frac{1\,mol\,O_2}{4\times96485\,C}\right)=0.070\,mol$$

$$V\left(O_2\right)=\left(\frac{\left(0.070\,mol\right)\times\left(0.082\,atm\cdot L\cdot K^{-1}\cdot mol^{-1}\right)\times\left(298\,K\right)}{\left(1.0\,atm\right)}\right)=1.7\,L \qquad V_{air}=8.6\,L$$

f)

$$\Delta_{rxn}G^\circ=\Delta_{rxn}H^\circ-T\Delta_{rxn}S^\circ$$

$$\Delta_{rxn}S^\circ=\left[2\times S^\circ\left(H_2O(l)\right)\right]-\left[2\times S^\circ\left(H_2(g)\right)+S^\circ\left(O_2(g)\right)\right]=2\times70.0-\left(2\times130.7+205.2\right)=$$
$$\Delta_{rxn}S^\circ=-326.6\,J\cdot mol^{-1}\cdot K^{-1}$$

$$\Delta_{rxn}H^\circ=\Delta_{rxn}G^\circ+T\Delta_{rxn}S^\circ=\left(-474\right)+298.15\times\left(+326.6\times10^{-3}\right)=-571.4\,kJ$$

maximum $w=\Delta_{rxn}G^\circ=-474\,kJ$

$$\eta=\frac{-474000\,J}{-571400\,J}=0.83$$

g)

$$\eta_{engine}=\frac{w}{q_H}=\frac{q_H-q_C}{q_H}=1-\frac{q_C}{q_H}$$

Since $\frac{q_H}{T_H}=\frac{q_H}{T_C}$ $\qquad \frac{q_C}{q_H}=\frac{T_C}{T_H}$

Thus; $\eta_{engine}=1-\frac{T_C}{T_H}$

$$0.83=1-\frac{313}{T_H} \qquad T_H=1.8\times10^{3}\,K\ \ or\ T_H=1.6\times10^{3}\,^\circ C$$