Chemical Equilbrium Notes after IRE analysis

CHEMICAL EQUILIBRIUM CALCULUATIONS

AT THIS POINT YOU SHOULD HAVE COMPLETED:

- I.R.E. ANALYSIS
- HOMEWORK ASSIGNMENT: H vs. S - ***min enthalpy and max entropy review***

THE EQUILIBRIUM CONSTANT

Consider the reaction $A + B \rightleftarrows C + D$

$aA + bB \rightleftarrows cC + dD$

(a , b, c, d coefficients used to balance the chem eqn)

RECALL FROM UNIT ONE:
Assuming one step reactions,

$v_f \propto [A]^a$

$v_f \propto [B]^b$ ***f = forward reaction***

$v_f \propto [A]^a [B]^b$

$v_f = k_f [A]^a [B]^b$

If the forward reaction is a one step reaction, then the reverse reaction is a one step reaction:

$v_r \propto [C]^c$

$v_r \propto [D]^d$ ***r = reverse reaction***

$v_r \propto [C]^c [D]^d$

$v_r = k_r [C]^c [D]^d$

AT CHEMICAL EQUILIBRIUM:

"conditions" of a reversible reaction @ EQUILIBRIUM

$v_f = v_r$

(RATE OF FORWARD RXN = RATE OF REVERSE RXN)

$k_f [A]^a [B]^b = k_r [C]^c [D]^d$

By convention:

$$K = \frac{k_f}{k_r}$$

$$\frac{k_f}{k_r} = \frac{[C]^c [D]^d}{[A]^a [B]^b}$$

- K sometimes seen as K_e or K_{eq}
- K is the product (multiplication) of the products raised to their coefficients divided by the product of the reactants raised to their coefficients
- K has no units: k_f and k_r units cancel.

Significance of K :

A large K value means the equilibrium lies to the right
OR in other words most of A and B will be converted to C and D. (favoured to the right).

FORWARD REACTION

$aA + bB \rightleftharpoons cC + dD$ large K value ← i.e. products favoured

$aA + bB \rightleftharpoons cC + dD$ small K value means reactants are favoured (reverse direction preferred)

Roughly speaking, a K value above one indicates the forward reaction is favoured more than the reverse.

The larger K gets, the more the reaction goes right. (and conversely for smaller).

K can NOT be a negative number!

QUESTION:

Derive from first principles, the constant K for : $H_2\,(g) + I_2\,(g) \rightleftarrows 2HI\,(g)$

$v_f \propto [H_2]^x$ $\quad v_r \propto [HI]^z$

$v_f \propto [I_2]^y$

$v_f \propto [H_2]^x [I_2]^y$

$v_f = k_f [H_2]^x [I_2]^y$ $\quad v_r = k_r [HI]^z$

← FOR THE PURPOSES OF K Value

✱ **ALWAYS ASSUME A ONE STEP REACTION** - ***this is called an elementary process!!***

Therefore the coefficients used to balance the equation are the exponents in the rate equation. (in Unit 1 we said that the coefficients used to balance the equation in the rate determining step are the exponents in the rate equation. We are assuming a one step mechanism, therefore the equation as written is the RDS.)

$v_f = k_f [H_2]^1 [I_2]^1$ $\quad v_r = k_r [HI]^2$

At equilibrium, $v_f = v_r$ (RATE OF FORWARD RXN = RATE OF REVERSE RXN)

$k_f [H_2] [I_2] = k_r [HI]^2$

$$K = \frac{k_f}{k_r} = \frac{[HI]^2}{[H_2][I_2]}$$

SEE SPECIAL "K" TRAITS NEXT PAGE (next document) Keq notes