

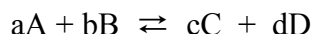
CHEMICAL EQUILIBRIUM CALCULATIONS

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 $A + B \rightleftharpoons C + D$



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

RECALL FROM UNIT ONE:

Assuming one step reactions,

$$v_f \cancel{\times} [A]^a$$

$$v_f \cancel{\times} [B]^b$$

$$v_f \cancel{\times} [A]^a [B]^b$$

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

f = forward reaction

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

$$v_r \cancel{\times} [C]^c$$

$$v_r \cancel{\times} [D]^d$$

$$v_r \cancel{\times} [C]^c [D]^d$$

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

r = reverse reaction

AT CHEMICAL 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:

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

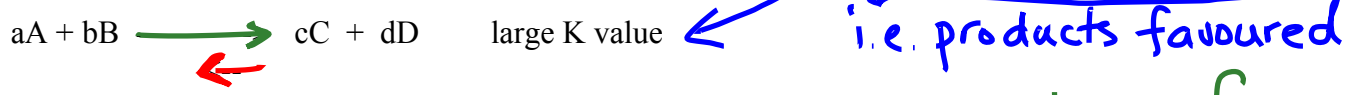
"conditions" of a reversible reaction @ EQUILIBRIUM

- 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.

FORWARD REACTION
(favoured to the right).



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 : $H_2(g) + I_2(g) \rightleftharpoons 2HI(g)$

$$v_f = k_f [H_2]^x [I_2]^y$$

$$v_r = k_r [HI]^z$$

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