Calculating Equilibrium Constant

- Example-1:

  1.000 mole of H_2 gas and 1.000 mole of I_2 vapor are introduced into a 5.00-liter sealed flask. The mixture is heated to a certain temperature and the following reaction occurs until equilibrium is established.

  $$H_2(g) + I_2(g) \rightleftarrows 2HI(g)$$

  At equilibrium, the mixture is found to contain 1.580 mole of HI. (a) What are the concentrations of H_2, I_2 and HI at equilibrium? (b) Calculate the equilibrium constant K_c.

Calculating Equilibrium Constant for reaction: $H_{2(g)} + I_{2(g)} \rightleftarrows 2HI_{(g)}$

	$H_2(g)$	+ $I_2(g)$	$\rightleftarrows$ 2 HI(g)
Initial [ ], M:	0.200	0.200	0.000
Change in [ ], M:	-0.158	-0.158	+ 0.316
Equilibrium [ ], M	0.042	0.042	0.316

$$K_c = \frac{[HI]^2}{[H_2][I_2]} = \frac{(0.316)^2}{(0.042)^2} = 57$$

Calculating Equilibrium Constant

- Example-2:

0.500 mole of HI is introduced into a 1.00 liter sealed flask and heated to a certain temperature. Under this condition HI decomposes to produce H_2 and I_2 until an equilibrium is established. An analysis of the equilibrium mixture shows that 0.105 mole of HI has decomposed. Calculate the equilibrium concentrations of H_2, I_2 and HI, and the equilibrium constant K_c for the following reaction:

$$H_{2(g)} + I_{2(g)} \rightleftarrows 2HI_{(g)},$$

Calculating Equilibrium Constant

- The reaction: $H_{2(g)}$ + $I_{2(g)}$ ⇄ $2HI_{(g)}$, proceeds from right to left.

	$H_2(g)$ +	$I_2(g)$ ⇄	$2HI(g)$
Initial [ ], *M*:	0.000	0.000	0.500
Change in [ ], *M*:	+0.0525	+0.0525	-0.105
Equilibrium [ ], *M*	0.0525	0.0525	0.395

$$K_c = \frac{(0.395)^2}{(0.0525)^2} = 56.6$$

THINGS WE STILL NEED TO TALK ABOUT

Vocabulary

- **Homogeneous equilibrium**: all the reactants and products are in the same phase
- **Heterogeneous equilibrium:** when there are two or more phases
- **Q_c**: reaction quotient, refers to a quotient obtained by applying the equilibrium law to initial concentrations (instead of equilibrium concentrations)

The Reaction Quotient

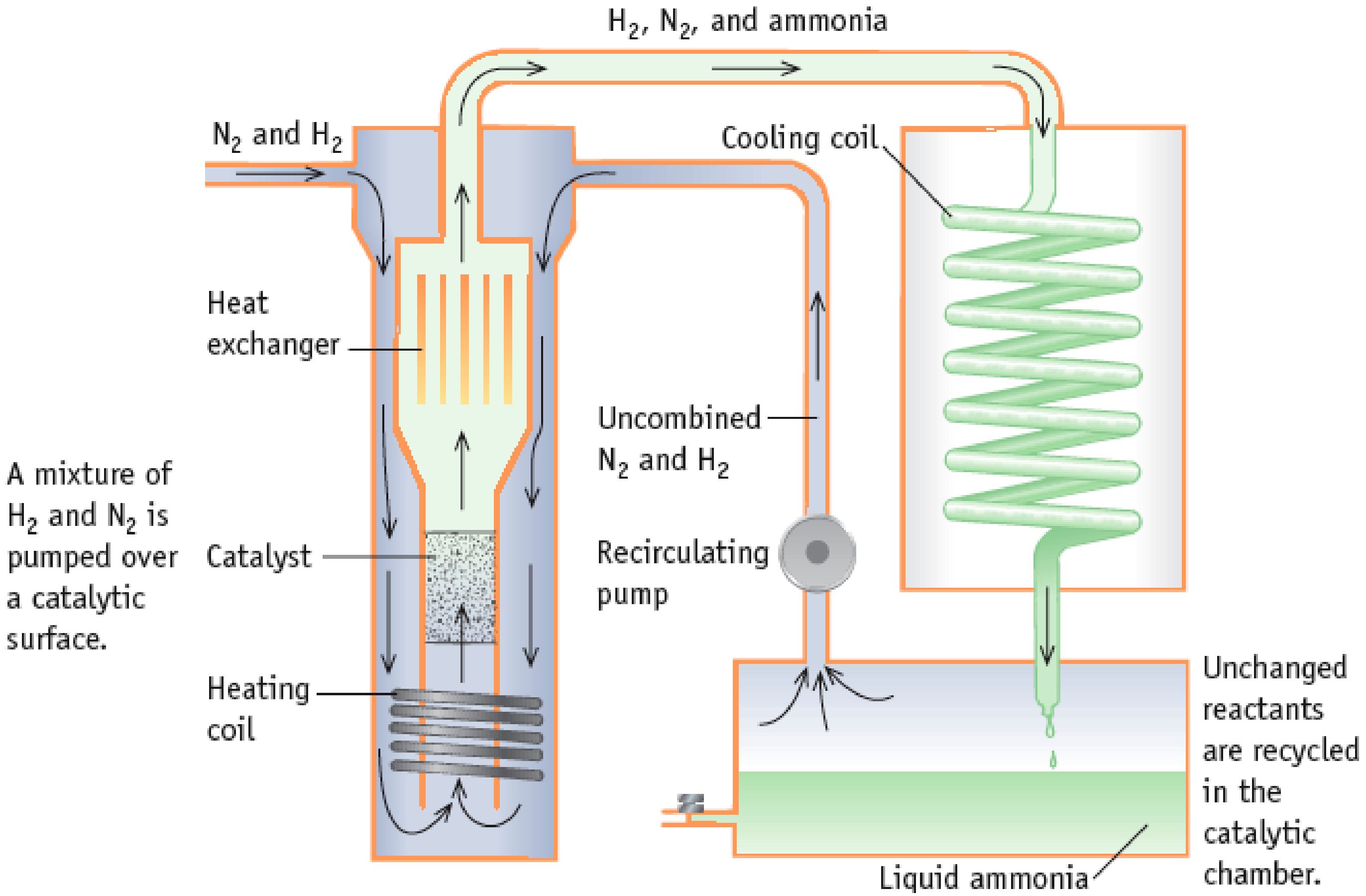
- The mass action expression or reaction quotient has the symbol Q.
  - Q has the same form as Kc
- The **major difference** between Q and Kc is that the concentrations used in Q are ***not necessarily equilibrium values.***
- Why do we need another "equilibrium constant" that does not use equilibrium concentrations?
- Q will help us predict how the equilibrium will respond to an applied stress.
- To make this prediction we compare Q with K_c.

The Reaction Quotient

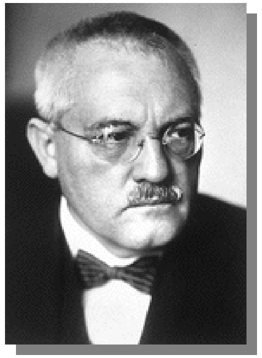
- The equilibrium constant for the following reaction is 49 at 450^{o}C. If 0.22 mole of I_2, 0.22 mole of H_2, and 0.66 mole of HI were put into an evacuated 1.00-liter container, would the system be at equilibrium? If not, what must occur to establish equilibrium?

The Haber Process: An Application of Equilibrium

- The Haber process is used for the commercial production of ammonia.
  - This is an enormous industrial process in the US and many other countries.
  - Ammonia is the starting material for fertilizer production.



Fritz Haber
1868-1934
Nobel Prize, 1918



Carl Bosch
1874-1940
Nobel Prize, 1931

ΔG, ΔG°, and K_{eq}

- ΔG is change in free energy at non-standard conditions.
- ΔG is related to ΔG°
- $\Delta G = \Delta G^\circ + RT \ln Q$

  where Q = reaction quotient
- When $Q < K$ or $Q > K$, reaction is spontaneous.
- When Q = K reaction is at equilibrium
- When $\Delta G = 0$ reaction is at equilibrium
- Therefore, $\Delta G^\circ = - RT \ln K$

Relationship Between ΔG^o_{rxn} and the Equilibrium Constant

- The relationships among ΔG^o_{rxn}, K, and the spontaneity of a reaction are:

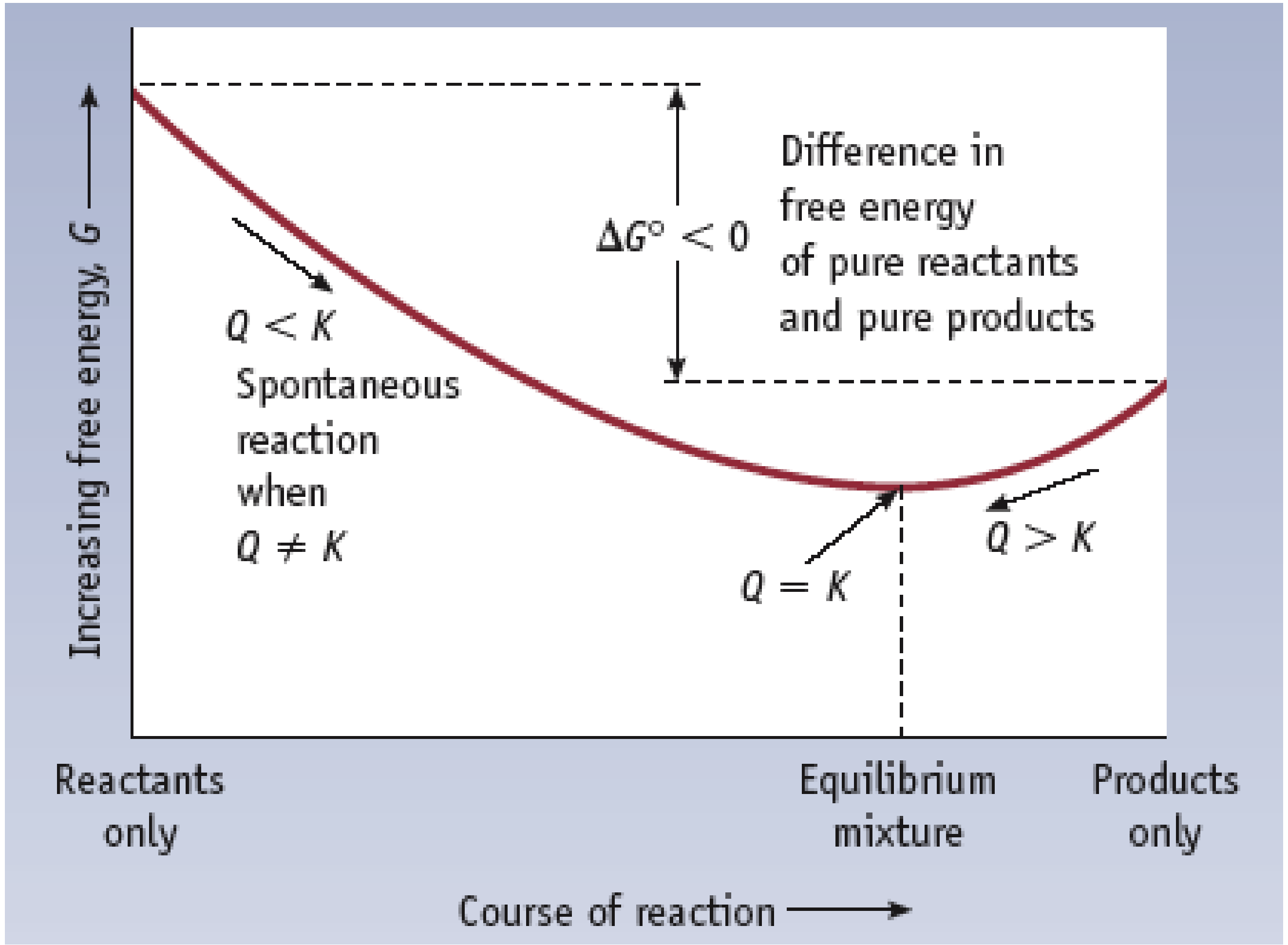
ΔG^o_{rxn}	K	Spontaneity at *unit* concentration
< 0	> 1	Forward reaction spontaneous
$= 0$	$= 1$	System at equilibrium
> 0	< 1	Reverse reaction spontaneous

ΔG, ΔG°, and K_{eq}

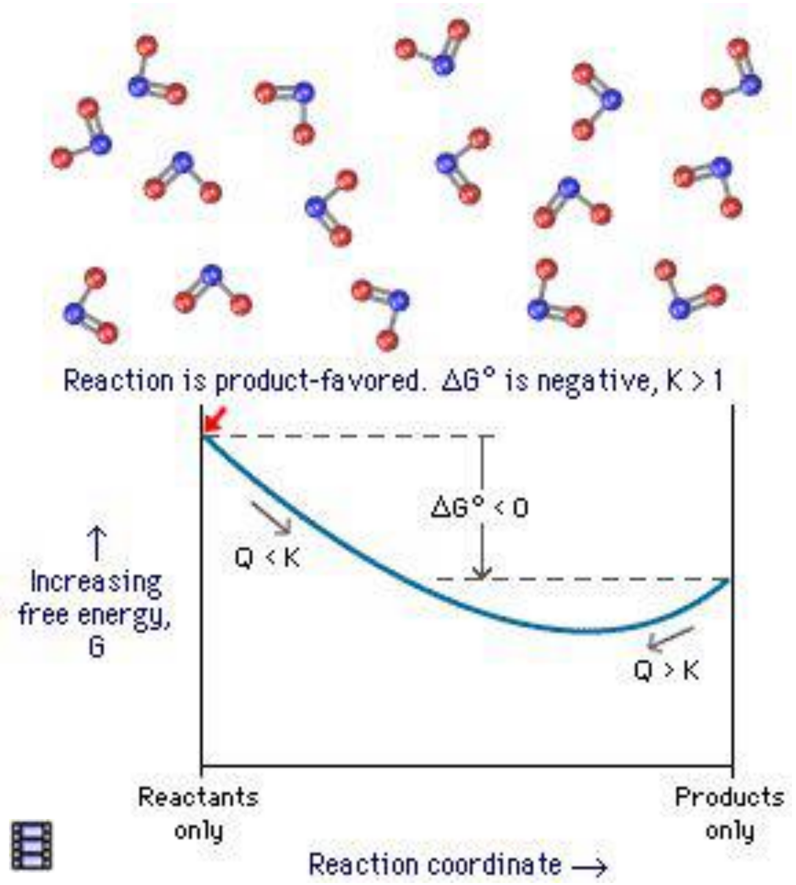
Product Favored, ΔG° negative, $K > 1$

But systems can reach equilibrium when reactants have NOT converted completely to products.

In this case ΔG_{rxn} is < ΔG^o_{rxn} , so state with both reactants and products present is MORE STABLE than complete conversion.



ΔG, ΔG°, and K_{eq}



- Product-favored
- 2 NO_2 ---> N_2O_4
- ΔG^o_{rxn} = – 4.8 kJ
- State with both reactants and products present is more stable than complete conversion.
- K > 1, more products than reactants.

Resources from the gas debate

- https://chemistry.stackexchange.com/questions/18567/what-would-be-the-effect-of-the-addition-of-an-inert-gas-to-a-reaction-at-equili#:~:text=at%20constant%20pressure%3A-,When%20an%20inert%20gas%20is%20added%20to%20the%20system%20in,number%20of%20moles%20of%20gases.
- http://ch302.cm.utexas.edu/chemEQ/equilibrium/selector.php?name=lechat-volume