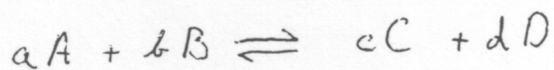


PREDICTING THE DIRECTION OF A REACTION

GIVEN A SET OF NON-EQUILIBRIUM CONCENTRATIONS

CALCULATE A NUMBER CALLED THE REACTION QUOTIENT Q_c

FOR A GENERAL REACTION



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

SO Q_c IS DEFINED EXACTLY AS K_c , EXCEPT NOT AT EQUILIBRIUM

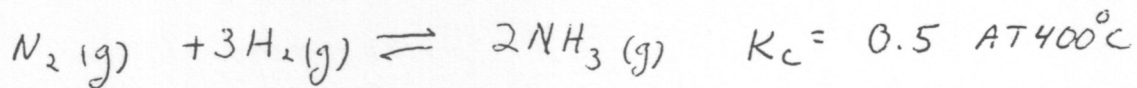
THEN COMPARE Q_c TO K_c USING THE FOLLOWING LOGIC

IF Q_c IS LARGER THAN K_c , REACTION GOES TOWARDS REACTANTS
REACTION GOES LEFT

IF Q_c IS SMALLER THAN K_c , REACTION GOES TOWARDS PRODUCTS
REACTION GOES RIGHT

IF Q_c IS = K_c , REACTION IS AT EQUILIBRIUM

EXAMPLE:



GIVEN CONDITIONS $[N_2] = 0.020 \text{ M}$ $[H_2] = 0.06 \text{ M}$ $[NH_3] = 0.01 \text{ M}$

$$Q_c = \frac{[NH_3]^2}{[N_2][H_2]^3} = \frac{0.01^2}{0.02 \times 0.06^3} = \frac{0.0001}{0.02 \times 0.00022}$$

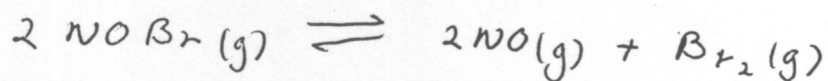
$$Q_c = \frac{0.0001}{0.0000043} = \frac{1}{0.043} = 23.1$$

OR

$$Q_c = \frac{1 \times 10^{-4}}{4.3 \times 10^{-6}} = .231 \times 10^2 = 23.1$$

23.1 IS GREATER THAN 0.5 SO REACTANTS ARE FAVORED

USING Q_c



AT 24°C $K_c = 3.07 \times 10^{-4}$

GIVEN THE CONDITIONS $[\text{NOBr}_2] = 0.06 \text{ M}$

$[\text{NO}] = 0.0151 \text{ M}$

$[\text{Br}_2] = 0.0108 \text{ M}$

CALCULATE Q_c AND PREDICT THE DIRECTION OF THE REACTION

$$Q_c = \frac{[\text{NO}]^2 [\text{Br}_2]}{[\text{NOBr}_2]^2}$$

$$Q_c = \frac{0.0151^2 \times 0.0108}{0.06^2}$$

$$Q_c = \frac{.000228 \times .0108}{.0036}$$

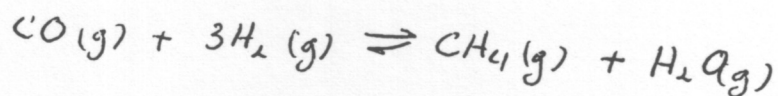
$$Q_c = \frac{.0000024}{.0036} \quad \text{OR} \quad \frac{2.4 \times 10^{-6}}{3.6 \times 10^{-3}}$$

$$Q_c = .000667 \quad \text{OR} \quad 6.67 \times 10^{-4}$$

$Q_c > K_c$ SO REACTION GOES TO LEFT

CALCULATING EQUILIBRIUM CONCENTRATIONS

GIVEN K_c AND ALL BUT ONE OF THE CONCENTRATIONS,
CALCULATE THE UNKNOWN CONCENTRATION



AT 1200°K $K_c = 3.92$ IF $[\text{CO}] = 0.30 \text{ M}$ WHAT IS $[\text{CH}_4]$?
 $[\text{H}_2] = 0.10 \text{ M}$
 $[\text{H}_2\text{O}] = 0.02 \text{ M}$

$$K_c = \frac{[CH_4][H_2O]}{[CO][H_2]^3}$$

SUBSTITUTE $3.92 = \frac{[CH_4][0.02]}{0.03 \times 0.1^3}$

SOLVE FOR

$$[CH_4] \quad [CH_4] = \frac{3.92 \times 0.03 \times 0.1^3}{0.02}$$

$$[CH_4] = 0.059 \text{ M}$$

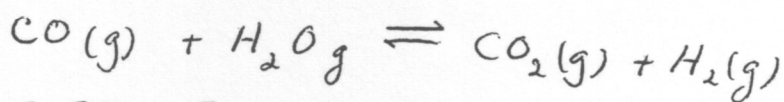
MORE CALCULATING EQUILIBRIUM CONCENTRATIONS

REMEMBER 1) SET UP A TABLE OF INITIAL, CHANGE AND FINAL CONCENTRATIONS

2) SUBSTITUTE KNOWN VALUES

3) SOLVE EQUILIBRIUM CONSTANT EQUATION

EXAMPLE:



AT 1000°C , $K_c = 0.58$, $[CO] = 0.020 \text{ M}$ $[H_2O] = 0.020 \text{ M}$

CONCENTRATIONS	CO	H ₂ O	CO ₂	H ₂
INITIAL	0.020 M	0.020 M	0	0
CHANGE	-x	-x	+x	+x
EQUILIBRIUM	0.020-x	0.020-x	x	x

$$K_c = \frac{[CO_2][H_2]}{[CO][H_2O]} = 0.58 = \frac{x \times x}{(0.020-x)(0.020-x)}$$

$$K_c = 0.58 = \frac{x^2}{(0.020-x)^2}$$

$$K_c = 0.58 = \frac{x^2}{(0.020 - x)^2}$$

TAKE THE SQUARE ROOT OF BOTH SIDES

$$0.76 = \frac{x}{0.020 - x}$$

SOLVE FOR X

$$x = (0.76)(0.020 - x)$$

DISTRIBUTE

$$x = 0.0152 - 0.76x$$

ADD $0.76x$ TO BOTH

$$1.76x = 0.0152$$

$$x = \frac{0.0152}{1.76} = 0.0086$$

SUBSTITUTE X INTO THE LAST ROW OF THE TABLE

CO	H ₂ O	CO ₂	H ₂
0.0114M	0.0114M	0.0086M	0.0086M

REVIEWING:

- 1) SET UP A TABLE OF CONCENTRATIONS
INITIAL CHANGE AND EQUILIBRIUM
- 2) SUBSTITUTE KNOWN VALUES AND EXPRESSIONS
IN X INTO THE EQUILIBRIUM CONSTANT
EXPRESSION
- 3) SOLVE THE EQUILIBRIUM CONSTANT EQUATION

CHANGING THE REACTION CONDITIONS

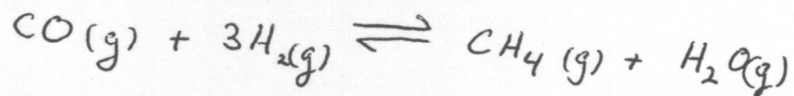
LE CHATELIER'S PRINCIPLE

WHEN A SYSTEM IN CHEMICAL EQUILIBRIUM IS DISTURBED BY A CHANGE OF TEMPERATURE, PRESSURE OR CONCENTRATION, THE SYSTEM SHIFTS IN EQUILIBRIUM COMPOSITION IN A WAY THAT TENDS TO COUNTERACT THIS CHANGE

REMOVING PRODUCTS OR ADDING REACTANTS

IT IS OFTEN POSSIBLE TO DRIVE A REACTION IN THE DESIRED DIRECTION BY EITHER REMOVING PRODUCT OR ADDING REACTANT. THE SYSTEM RESPONDS TO PRODUCT REMOVAL BY RE-ESTABLISHING EQUILIBRIUM BY MAKING MORE PRODUCT.

IN THIS REACTION

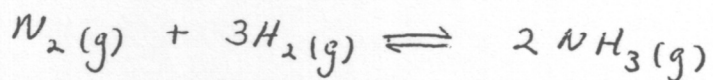


WATER VAPOR IS EASILY REMOVED FROM THE REACTION MIXTURE BY COOLING. ONCE THE H_2O IS REMOVED, LE CHATELIER'S PRINCIPLE PREDICTS THAT THE REACTION WILL GO IN A FORWARD DIRECTION UNTIL EQUILIBRIUM IS RE-ESTABLISHED.

THIS TABLE (14-1) SHOWS THIS EFFECT

ORIGINAL MIXTURE	CO	H ₂	CH ₄	H ₂ O
	0.613	1.839	0.387	0.387
AFTER H ₂ O REMOVAL (BEFORE EQUILIB)	0.613	1.839	0.387	0
NEW EQUILIBRIUM	0.491	1.473	0.509	0.122

INSTEAD OF REMOVING PRODUCT, REACTANT CAN BE ADDED
IN THIS REACTION:



IT IS POSSIBLE TO ADD SOME (CHEAP) N_2 TO AN EQUILIBRIUM
MIXTURE. LECHATELIER'S PRINCIPLE PREDICTS THAT THE REACTION
WILL GO IN THE FORWARD DIRECTION AND MAKE MORE NH_3

TO SUM UP, LECHATELIER'S PRINCIPLE SAYS THAT:

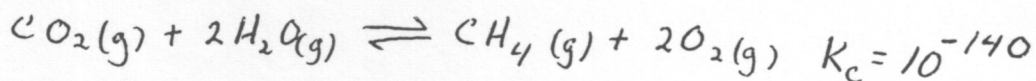
WHEN MORE REACTANT IS ADDED, OR SOME PRODUCT
IS REMOVED, (AND THE CONCENTRATIONS OF PRODUCT OR
REACTANT ARE CHANGED) NET REACTION OCCURS FROM
LEFT TO RIGHT (FORWARD) TO GIVE A NEW EQUILIBRIUM
AND MORE PRODUCTS ARE PRODUCED

CONVERSELY

WHEN MORE PRODUCT IS ADDED, OR SOME REACTANT
IS REMOVED FROM AN EQUILIBRIUM MIXTURE, (AND THE
CONCENTRATIONS OF PRODUCT OR REACTANT ARE CHANGED)
NET REACTION OCCURS FROM RIGHT TO LEFT (REVERSE)
TO GIVE A NEW EQUILIBRIUM, AND MORE REACTANTS ARE
PRODUCED

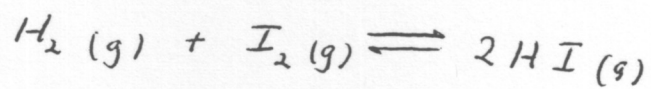
KEEP IN MIND THAT A REACTION WHOSE EQUILIBRIUM CONSTANT
IS EXTREMELY SMALL REMAINS ALMOST COMPLETELY AS
REACTANTS AND CANNOT BE MUCH AFFECTED BY ADDING
REACTANTS OR REMOVING PRODUCTS

EXAMPLE

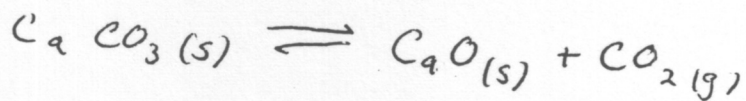


LE CHATELIER'S EXAMPLES

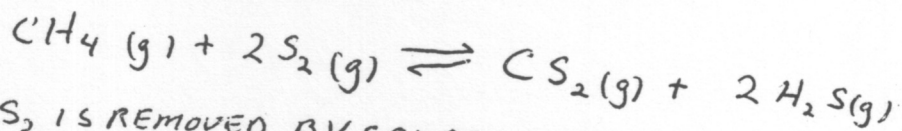
PREDICT THE DIRECTION IF:



IF H_2 IS REMOVED



IF THE PRESSURE [CONCENTRATION] OF CO_2 IS INCREASED

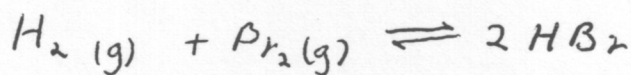


IF CS_2 IS REMOVED BY CONDENSATION

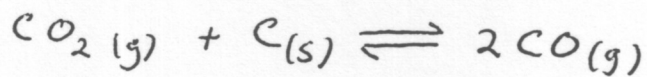
FOR GASSES, PARTIAL PRESSURE IS EQUIVALENT TO CONCENTRATION
A SIMPLE SUMMARY OF LE CHATELIER'S PRINCIPLE FOR GASSES
IS:

IF THE PRESSURE IS INCREASED BY DECREASING THE
VOLUME (COMPRESSING) A REACTION MIXTURE, THE REACTION
SHIFTS IN THE DIRECTION OF OF FEWER MOLES OF GAS

EXAMPLES



IF PRESSURE IS INCREASED, GOES TO



IF PRESSURE IS INCREASED, GOES TO

EFFECT OF TEMPERATURE CHANGE

LE CHATELIER'S PRINCIPLE FOR TEMPERATURE CHANGES IS EASILY UNDERSTOOD IF YOU CONSIDER HEAT AS A PRODUCT OF A REACTION (OR A REACTANT)

EXOTHERMIC REACTIONS PRODUCE HEAT.

INCREASING THE TEMPERATURE DECREASES PRODUCTS K_c SMALL

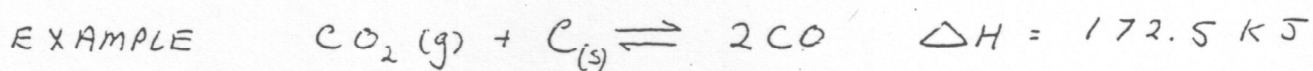
DECREASING THE TEMPERATURE INCREASES PRODUCTS K_c LARGE

THE OPPOSITE IS TRUE OF ENDOTHERMIC REACTIONS

ENDOTHERMIC REACTIONS CONSUME HEAT

INCREASING THE TEMPERATURE INCREASES PRODUCTS K_c LARGER

DECREASING THE TEMPERATURE DECREASES PRODUCTS K_c SMALLER



IS A HIGH OR LOW TEMPERATURE MORE FAVORABLE TO THE FORMATION OF CARBON MONOXIDE?

IS THE REACTION ENDO OR EXOTHERMIC?