**Worksheet: Chemical equilibrium in the Haber Process**

**Name(s)**

This experiment calculates chemical equilibrium constants for the gas-phase Haber reaction  
(N2 + 3H2 🡪 2NH3) from measurements of equilibrium concentrations. The heat of reaction is determined by measuring the equilibrium constant over a range of temperatures.

**Student learning objectives**

1. Be able to calculate an equilibrium constant from equilibrium concentrations.
2. Be able apply the van Hoff equation to determine the heat of reaction.

**Equipment**

This catalytic reaction takes place at high pressures and elevated temperatures. Hydrogen and nitrogen are fed to the reactor to form ammonia. Ammonia can also be added to the reactor feed since in commercial reactors, the unreacted N2 and H2 are recycled back to the feed and the recycle stream contains some NH3. A gas chromatograph measures the composition of the outlet stream from the reactor.

A diagram of a gas tank

AI-generated content may be incorrect.

**Questions to answer before starting the experiment**

How does the equilibrium constant change with temperature for an exothermic reaction? Explain.

How does the equilibrium constant change with pressure for a gas-phase reaction?

What are the units of an equilibrium constant?

**Before starting**

1. Set the temperature of the sand bath heater by clicking on the up or down arrows. Record the temperature in Table 1 below.
2. Click the valves on top of the H2 and N2 tanks to open the tanks.
3. Optionally, click the valve to open the NH3 tank. Record the mass flow rate in Table 1.
4. Open the valve on top of the He tank. The He flow feeds a sample of gas into the gas chromatograph to measure the composition of the gas leaving the reactor.
5. Select an operating pressure using the up and down arrows on the pressure gauge/controller. Record the pressure in Table 1.
6. Select the flow rates using the up and down arrows on the mass flow controllers. Record in Table 1 the mass flow rates to the reactor. Calculate the molar flow rates and record in Table 1.
7. When the system starts up, the effluent from the reactor flows to a vent.
8. Allow time for the system to reach equilibrium; the GC screen should read READY FOR SAMPLE.
9. Switch the valve (**how**?) to take a sample and inject it into the GC.
10. Record in Table 2 below the mole fraction of NH3 obtained by the GC.
11. Calculate the mole fractions of N2 and H2 in the effluent using the feed composition and stoichiometry and record in Table 2.
12. Calculate the equilibrium pressures and record in Table 2
13. Calculate the equilibrium constant and record in Table 2

In this equation, the pressure is in units of bar, and the equation is usually written as indicated below, where the pressures must be in bar and the equilibrium constant is dimensionless.

This equation assumes ideal gases, which is not correct at the high pressures used for ammonia formation, but this assumption simplifies the calculations.

Repeat these measurements for a range of temperatures and pressures and record in Tables 1 & 2.

**Table 1 Feed conditions**

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  |  |  | Feed rates (mg/min) | | | Feed rates (mol/min) | | |  |
| Experiment | Temperature (K) | Pressure (bar) | N2 | H2 | NH3 | N2 | H2 | NH3 |  |
| #1 |  |  |  |  |  |  |  |  |  |
| #2 |  |  |  |  |  |  |  |  |  |
| #3 |  |  |  |  |  |  |  |  |  |
| #4 |  |  |  |  |  |  |  |  |  |
| #5 |  |  |  |  |  |  |  |  |  |
| #6 |  |  |  |  |  |  |  |  |  |
| #7 |  |  |  |  |  |  |  |  |  |
| #8 |  |  |  |  |  |  |  |  |  |
| #9 |  |  |  |  |  |  |  |  |  |

**2 Equilibrium conditions**

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  |  |  | Equil. composition | | | Equilibrium pressure (bar) | | | Keq |
| Experiment | T (K) | P (bar) | NH3 | N2 | H2 | PN2 | PH2 | PNH3 |  |
| #1 |  |  |  |  |  |  |  |  |  |
| #2 |  |  |  |  |  |  |  |  |  |
| #3 |  |  |  |  |  |  |  |  |  |
| #4 |  |  |  |  |  |  |  |  |  |
| #5 |  |  |  |  |  |  |  |  |  |
| #6 |  |  |  |  |  |  |  |  |  |
| #7 |  |  |  |  |  |  |  |  |  |
| #8 |  |  |  |  |  |  |  |  |  |
| #9 |  |  |  |  |  |  |  |  |  |

What can you conclude about the effect of pressure on the equilibrium constant?

**Data Analysis:**

Plot ln(Keq) versus inverse temperature.

Can the data be fit by a straight line?

Calculate the heat of reaction from the van Hoff equation, using all your data.

where K2 (dimensionless) is the equilibrium constant at temperature T2

K1 (dimensionless) is the equilibrium constant at temperature T1

T1 and T2 are absolute temperatures (K)

= heat of reaction (J/mol)

R = ideal gas constant (J/mol K)

= J/mol = kJ/mol

**Questions to answer**

1. Where might these measurements have errors?
2. What safety precautions would you take to conduct this experiment in the laboratory?