

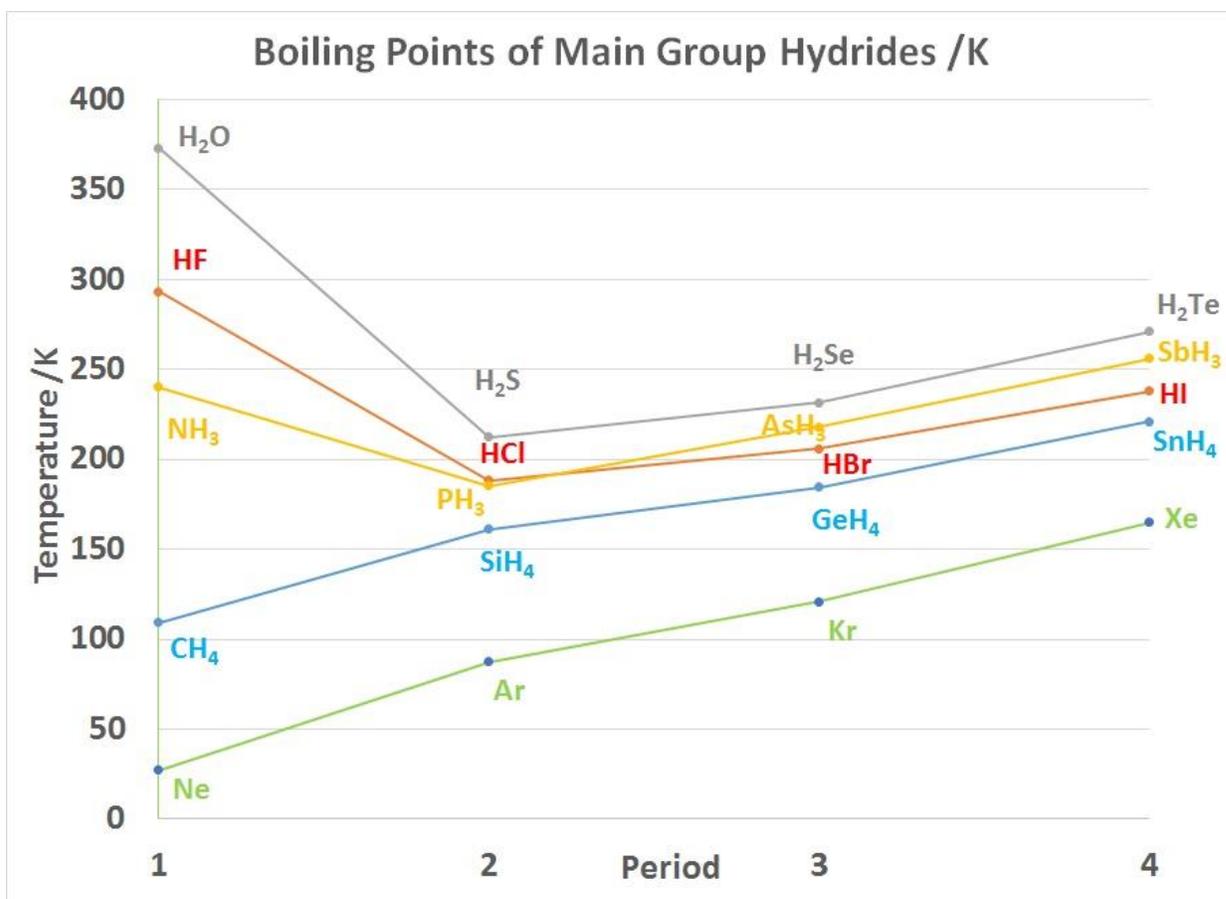
HYDROGEN BONDS : A STUDY

A hydrogen bond is the name given to the electrostatic attraction between polar molecules that occurs when a hydrogen (H) atom bound to a highly electronegative atom such as nitrogen (N), oxygen (O) or fluorine (F) experiences attraction to some other nearby highly electronegative atom. The name is something of a misnomer, as it represents a particularly strong dipole-dipole attraction, rather than a typical covalent bond.

The 2011 IUPAC definition specifies that "*The hydrogen bond is an attractive interaction between a hydrogen atom from a molecule or a molecular fragment X-H in which X is more electronegative than H, and an atom or a group of atoms in the same or a different molecule, in which there is evidence of bond formation.*"

These hydrogen-bond attractions can occur between molecules (intermolecular) or within different parts of a single molecule (intramolecular). The hydrogen bond (5 to 30 kJ/mole) is stronger than a van der Waals interaction, but weaker than covalent or ionic bonds. This type of bond can occur in inorganic molecules such as water and in organic molecules like DNA and proteins.

Intermolecular hydrogen bonding is responsible for the high boiling point of water (100 °C) compared to the other group 16 hydrides that have no hydrogen bonds. Intramolecular hydrogen bonding is partly responsible for the secondary and tertiary structures of proteins and nucleic acids. It plays an important role in the structure of polymers, both synthetic and natural.

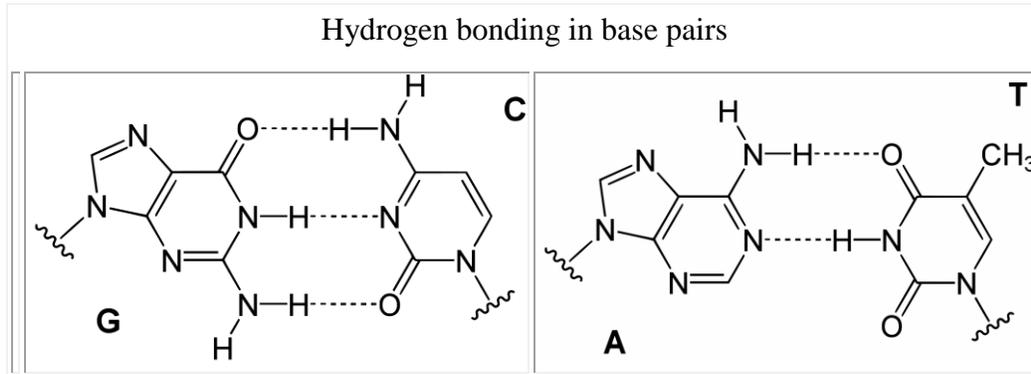


BP's of MG hydrides with Noble gases for comparison /K

Hydrogen bonding in biological systems.

[Base pairs](#), which form between specific nucleobases (also termed nitrogenous bases), are the building blocks of the DNA double helix and contribute to the folded structure of both DNA and RNA. Dictated by specific hydrogen bonding patterns, Watson-Crick base pairs (guanine-cytosine and adenine-thymine) allow the DNA helix to maintain a regular helical structure that is subtly dependent on its nucleotide sequence. The complementary nature of this based-paired structure provides a backup copy of all genetic information encoded within double-stranded DNA. The regular structure and data redundancy provided by the DNA double helix make DNA well suited to the storage of genetic information, while base-pairing between DNA and incoming nucleotides provides the mechanism through which DNA polymerase replicates DNA, and RNA polymerase transcribes DNA into

RNA. Many DNA-binding proteins can recognize specific base pairing patterns that identify particular regulatory regions of genes.



Applications of hydrogen

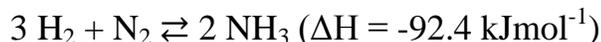
Large quantities of H_2 are used by the petroleum and chemical industries. The largest application of H_2 is for the processing ("upgrading") of fossil fuels, and in the production of ammonia. The key consumers of H_2 in the petrochemical plant include hydrodealkylation, hydrodesulfurization, and hydrocracking. H_2 has several other important uses. H_2 is used as a hydrogenating agent, particularly in increasing the level of saturation of unsaturated fats and oils (found in items such as margarine), and in the production of methanol. It is similarly the source of hydrogen in the manufacture of hydrochloric acid. H_2 is used as a reducing agent of metallic ores.

Nitrogen is a strong limiting nutrient in plant growth. Carbon and oxygen are also critical, but are more easily obtained by plants from soil and air. Even though air is 78% nitrogen, atmospheric nitrogen is nutritionally unavailable because nitrogen molecules are held together by strong triple bonds. Nitrogen must be 'fixed', i.e. converted into some bioavailable form, through natural or man-made processes. It was not until the early 20th century that Fritz Haber developed the first practical process to convert atmospheric

nitrogen to ammonia, which is nutritionally available.

Fertilizer generated from ammonia produced by the [Haber](#) process is estimated to be responsible for sustaining one-third of the Earth's population. It is estimated that half of the protein within human beings is made of nitrogen that was originally fixed by this process; the remainder was produced by nitrogen fixing [bacteria and archaea](#).

Dozens of chemical plants worldwide produce [ammonia](#), consuming more than 1% of all man-made power. Ammonia production is thus a significant component of the world energy budget. Modern ammonia-producing plants depend on industrial hydrogen production to react with atmospheric nitrogen using a magnetite catalyst or over a promoted Fe catalyst under high pressure (100 standard atmospheres (10,000 kPa)) and temperature (450 °C) to form anhydrous liquid ammonia. This step is known as the ammonia synthesis loop (also referred to as the [Haber-Bosch process](#)):

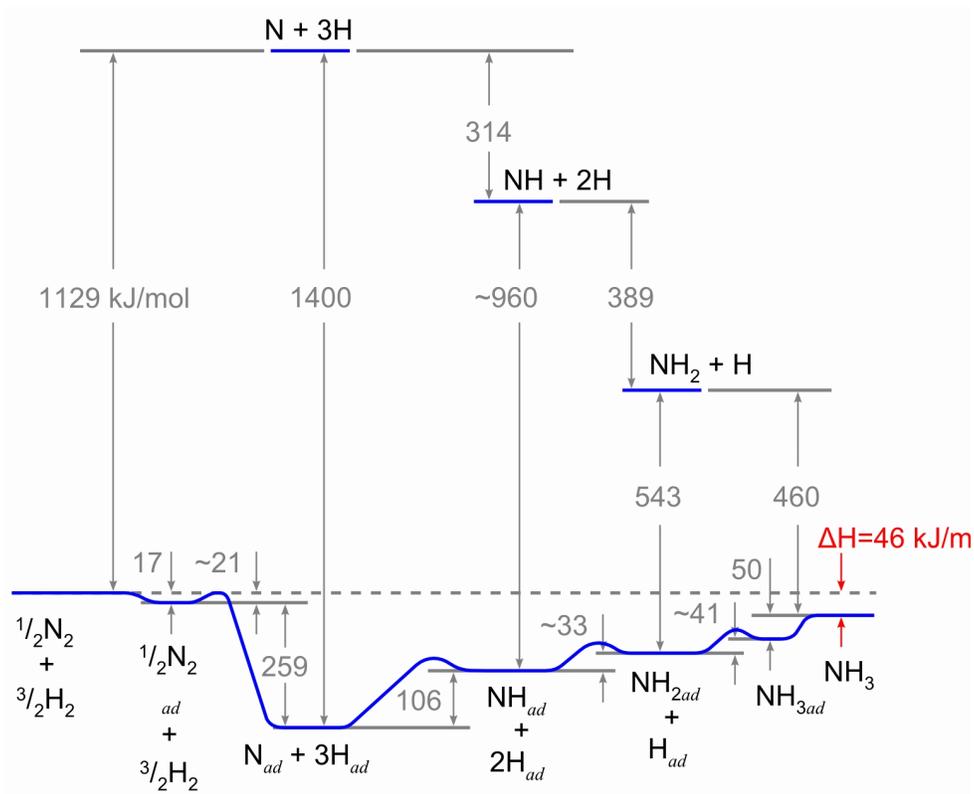


Nitrogen (N₂) is very unreactive because the molecules are held together by strong triple bonds. The Haber process relies on catalysts that accelerate the cleavage of this triple bond.

At room temperature, the equilibrium is strongly in favor of ammonia, but the reaction doesn't proceed at a detectable rate. Thus two opposing considerations are relevant to this synthesis. One possible solution is to raise the temperature, but because the reaction is exothermic, the equilibrium quickly becomes quite unfavourable at atmospheric pressure. Low temperatures are not an option since the catalyst requires a temperature of at least 400 °C to be efficient. By increasing the pressure to around 200 atm the equilibrium concentrations are altered to give a profitable yield.

The reaction scheme, involving the heterogeneous catalyst, is believed to involve the following steps:

1. $\text{N}_2(\text{g}) \rightarrow \text{N}_2(\text{adsorbed})$
2. $\text{N}_2(\text{adsorbed}) \rightarrow 2\text{N}(\text{adsorbed})$
3. $\text{H}_2(\text{g}) \rightarrow \text{H}_2(\text{adsorbed})$
4. $\text{H}_2(\text{adsorbed}) \rightarrow 2\text{H}(\text{adsorbed})$
5. $\text{N}(\text{adsorbed}) + 3\text{H}(\text{adsorbed}) \rightarrow \text{NH}_3(\text{adsorbed})$
6. $\text{NH}_3(\text{adsorbed}) \rightarrow \text{NH}_3(\text{g})$



Reaction 5 actually consists of three steps, forming NH , NH_2 , and then NH_3 . Experimental evidence suggests that reaction 2 is the slow, rate-determining step. This is not unexpected given that the bond broken, the nitrogen triple bond, is the strongest of the bonds that must be broken.

Source : http://wwwchem.uwimona.edu.jm:1104/courses/CHEM1902/IC10K_MG_hydrogen.html