Hydrogen Atom

Pradeep Kumar, Mamta, Deepika

Abstract **Hydrogen atom is an atom of the chemical element hydrogen. The electrically neutral atom contains a single positively charged proton and a single negatively charged electron bound to the nucleus by the Coulomb force. Atomic hydrogen constitutes about 75% of the elemental (baryonic) mass of the universe.[1]**

In everyday life on Earth, isolated hydrogen atoms (usually called "atomic hydrogen" or, more precisely, "monatomic hydrogen") are extremely rare. Instead, hydrogen tends to combine with other atoms in compounds, or with itself to form ordinary (diatomic) hydrogen gas, H2. "Atomic hydrogen" and "hydrogen atom" in ordinary English use have overlapping, yet distinct, meanings. For example, a water molecule contains two hydrogen atoms, but does not contain atomic hydrogen (which would refer to isolated hydrogen atoms).

Keywords— Hydrogen Atoms.

I. INTRODUCTION

The H–H bond is one of the strongest bonds in chemistry, with a bond dissociation enthalpy of 435.88 kJ/mol at 298 K (25 °C; 77 °F). As a consequence of this strong bond, H2 dissociates to only a minor extent until higher temperatures. At 3,000 K (2,730 °C; 4,940 °F), the degree of dissociation is just 7.85%:[2]

$H_2 \rightleftharpoons 2\,H$

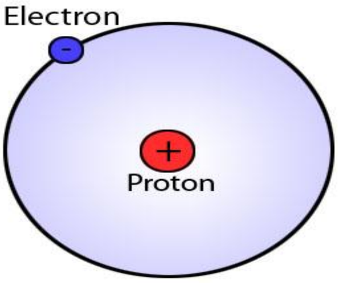
Hydrogen atoms are so reactive that they combine chemically with almost all elements.

The most abundant isotope, hydrogen-1, protium, or light hydrogen, contains no neutrons; other isotopes of hydrogen, such as deuterium or tritium, contain one or more neutrons. The formulas below are valid for all three isotopes of hydrogen, but slightly different values of the Rydberg constant (correction formula given below) must be used for each hydrogen isotope.

II. PROBABILITY DENSITY

The image to the right shows the first few hydrogen atom orbitals (energy eigenfunctions). These are cross-sections of the probability density that are color-coded (black represents zero density and white represents the highest density). The angular momentum (orbital) quantum number ℓ is denoted in each column, using the usual spectroscopic letter code (*s*means $\ell = 0$, *p* means $\ell = 1$, *d* means $\ell = 2$). The main (principal) quantum number *n* (= 1, 2, 3, ...) is marked to the right of each row. For all pictures the magnetic quantum number *m* has been set to 0, and the cross-sectional plane is the *xz*-plane (*z* is the vertical axis). The probability density in three-dimensional space is obtained by rotating the one shown here around the *z*-axis.

Fluorescence occurs when an excited electron relaxes to the ground state and combines with the hole. In a simplified model, the energy of the emitted photon can be understood as the sum of the band gap energy between the occupied level and the unoccupied energy level, the confinement energies of the hole and the excited electron, and the bound energy of the exciton (the electron-hole pair):



The hydrogen atom consists of a proton of mass mp=1.7´10-27kg and charge qe=1.6´10-19C and an electron of mass me=9.1´10-31kg and charge -qe. The dominant part of the interaction between the two particles is the electrostatic interaction.

Problem:

In the interstellar medium electrons may recombine with protons to form hydrogen atoms with high principal quantum numbers. A transition between successive values of n gives rise to a recombination line.

(a) A radio recombination line occurs at 5.425978 * 1010 Hz for a n = 50 to n = 49 transition. Calculate the Rydberg constant for H.

(b) Compute the frequency of the H recombination line corresponding to the transition n = 100 to n = 99

III HYDROGEN ATOM ORBITALS

When a planet moves around the sun, you can plot a definite path for it which is called an orbit. A simple view of the atom looks similar and you may have pictured the electrons as orbiting around the nucleus.

The truth is different, and electrons in fact inhabit regions of space known as orbitals.

Orbits and orbitals sound similar, but they have quite different meanings. It is essential that you understand the difference between them.

The impossibility of drawing orbits for electrons.

To plot a path for something you need to know exactly where the object is and be able to work out exactly where it's going to be an instant later. You can't do this for electrons.

The Heisenberg Uncertainty Principle says - loosely - that you can't know with certainty both where an electron is and where it's going next. (What it actually says is that it is impossible to define with absolute precision, at the same time, both the position and the momentum of an electron.)

That makes it impossible to plot an orbit for an electron around a nucleus. Is this a big problem? No. If something is impossible, you have to accept it and find a way around it.

These are cross-sections of the probability density that are color-coded (black represents zero density and white represents the highest density). The angular momentum (orbital) quantum number ℓ is denoted in each column, using the usual spectroscopic letter code (s means ℓ = 0, p means ℓ = 1, d means ℓ = 2). The main (principal) quantum number n (= 1, 2, 3, ...) is marked to the right of each row. For all pictures the magnetic quantum number m has been set to 0, and the cross-sectional plane is the xz-plane (z is the vertical axis). The probability density in three-dimensional space is obtained by rotating the one shown here around the z-axis.

The "ground state", i.e. the state of lowest energy, in which the electron is usually found, is the first one, the 1s state (principal quantum level n = 1, ℓ = 0).

An image with more orbitals is also available (up to higher numbers n and ℓ).

Black lines occur in each but the first orbital: these are the nodes of the wavefunction, i.e. where the probability density is zero. (More precisely, the nodes are spherical harmonics that appear as a result of solving Schrödinger's equation in polar coordinates.)

IV. D AND F ORBITALS

In addition to s and p orbitals, there are two other sets of orbitals which become available for electrons to inhabit at higher energy levels. At the third level, there is a set of five d orbitals (with complicated shapes and names) as well as the 3s and 3p orbitals (3px, 3py, 3pz). At the third level there are a total of nine orbitals altogether.

At the fourth level, as well the 4s and 4p and 4d orbitals there are an additional seven f orbitals - 16 orbitals in all. s, p, d and f orbitals are then available at all higher energy levels as well.

For the moment, you need to be aware that there are sets of five d orbitals at levels from the third level upwards, but you probably won't be expected to draw them or name them. Apart from a passing reference, you won't come across f orbitals at all.
The electron configuration of an atom shows the number of electrons in each sublevel in each energy level of the ground-state atom. To determine the electron configuration of a particular atom, start at the nucleus and add electrons one by one until the number of electrons equals the number of protons in the nucleus. Each added electron is assigned to the lowest-energy sublevel available. The first sublevel filled will be the 1s sublevel, then the 2s sublevel, the 2p sublevel, the 3s, 3p, 4s, 3d, and so on. This order is difficult to remember and often hard to determine from energy-level diagrams

A more convenient way to remember the order.The principal energy levels are listed in columns, starting at the left with the 1s level. To use this figure, read along the diagonal lines in the direction of the arrow. The order is summarized under the diagram.

When the electron is in a definite energy level we shall refer to the Pn distributions as electron density distributions, since they describe the manner in which the total electronic charge is distributed in space. The electron density is expressed in terms of the number of electronic charges per unit volume of space, e-/V. The volume V is usually expressed in atomic units of length cubed, and one atomic unit of electron density is then e-/a03. To give an idea of the order of magnitude of an atomic density unit, 1 au of charge density e-/a03 = 6.7 electronic charges per cubic Ångstrom. That is, a cube with a length of 0.52917 ´10-8 cm, if uniformly filled with an electronic charge density of 1 au, would contain 6.7 electronic charges.

P1 may be represented in another manner. Rather than considering the amount of electronic charge in one particular small element of space, we may determine the total amount of charge lying within a thin spherical shell of space. Since the distribution is independent of direction, consider adding up all the charge density which lies within a volume of space bounded by an inner sphere of radius r and an outer concentric sphere with a radius only infinitesimally greater, say r + Dr. The area of the inner sphere is 4pr2 and the thickness of the shell is Dr. Thus the volume of the shell is 4pr2 Dr (Click here for note.) and the product of this volume and the charge density P1(r), which is the charge or number of electrons per unit volume, is therefore the total amount of electronic charge lying between the spheres of radius r and r + Dr. The product 4pr2Pn is given a special name, the radial distribution function, which we shall label Qn(r).

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