Oxygen Lone-Pair Electrons behind Amazing Properties of Water-Electrolysis Gas-Mixture

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The mixture of gasses evolving from water electrolysis, referred to by some as Brown's gas, has some unusual characteristics defying current Chemistry but can be understood by involving the lone pair electrons of oxygen. The SP^3 hybridization creates four equivalent electron orbitals for oxygen atom, two bond-pair and two lone-pair. The energy levels of the bond-pair electron are widely and unevenly spaced. The lone-pair electrons, in contrast, have narrow and equi-spaced energy levels. A bond-pair electron when excited to higher energy returns to the ground state immediately. The lone-pair electron however stays in its higher energy state for long. The cation H^+ is neutralized at the cathode to liberate mono-atomic (H) and diatomic (H_2) hydrogen gas. The anion OH^- is oxidized at the anode to produce mono-atomic (O) and diatomic (O_2) oxygen gas and water (H_2O) vapor plus electrons (e^-), which are transported externally to the cathode. The electrical energy of electrolysis promotes the lone-pair electrons of oxygen atoms to higher energy levels in the oxygen gas (O, O_2) and in water (H_2O) vapor. Since the energy difference ΔE between adjacent levels is small the life time Δt, related by $\Delta E \cdot \Delta t \geq \hbar$, is long to keep them stay promoted for a long time even after electrolysis. This increases the latent heat of combustion of the water-electrolysis gas-mixture, which though cool at about 130°C (266°F) can melt metals. When the electrolysis gas torch is directed to liquid water, gas's water vapor component quietly dissolves un-burnt without producing enough heat to boil the liquid water. But water does boil if the gas torch heats the container from outside. The gas mixture burns in vacuum because no oxygen is needed from outside. No other theory, past or current, is so natural and explanatory.

1. What is the Water-electrolysis Gas-Mixture?

This author came to know about Brown's Gas and its amazing characteristics from the videoconference "Characterizing Brown's Gas' given by Chris Eckman [1] Saturday 19 December 2009 under the aegis of the Natural Philosophy Alliance. Yull Brown gave many public demonstrations and got his own patents (4,010,777 and 4,081,656) in 1974. Dr. Rhodes received the US patent 3262872 in 1966 and 3310483 later for the methods of producing this, what he called 'the single ducted' oxy-hydrogen gas, distinctly different from the usual hydrogen torch with two hoses, one for hydrogen and the other for oxygen. In 1990s George Wiseman (http://www.eagle-research.com/) defined it as 'the entire mixture of gasses evolving from a water electrolyzer without separating the resulting gasses'. According to Santilli (http://www.magnegas.com/) researching since 1970s, it is a mixture of monatomic and diatomic hydrogen and oxygen and a special form of water called Electrically Expanded Water (EEW) or Magnecule HHO. Chris Eckman (cryptoscientia@gmail.com) holds similar views. In this present paper we take it as the mixture of mono- and di-atomic hydrogen and oxygen gasses plus water vapor evolved during electrolysis of 'double glass-distilled pure water' free from all contaminations appearing in the mass spectrometric analysis of Chris Eckman. [1] However, the lone-pair electrons of oxygen atoms in the oxygen gas and in the water vapor molecules are promoted to higher energy levels by the electrical energy (see below). To raise the conductivity of water under electrolysis a little Sodium Hydroxide (NaOH), Potassium Hydroxide (KOH) or Sulphuric acid (H_2SO_4) is added to it.

2. The Theories Proposed

Yull Brown was the first to offer an explanation but his 'fluid crystal' theory died out long ago. Santilli has theorized that the two hydrogen atoms squeeze together to produce an isomer of the water molecule. Getting a cue from Santilli, Chris Eckman also favors an isomer of water molecule, the 'linear molecule', but he himself is not completely satisfied with it. [1] This justifies the search for an alternative new theory involving lone pair electrons of oxygen.

3. The Significance of Lone-pair & Bond-pair Electrons

The electronic structure of oxygen atom in its ground state is $1s^2\ 2s^2\ 2p_x^2\ 2p_y^1\ 2p_z^1$ as shown in Figure-1 A, upper. The two unpaired electrons in the $2p_y^1$, $2p_z^1$ orbitals could form covalent bonds with hydrogen atoms H to give a *linear* and *non-polar* molecule H-O-H of water like F-Be-F molecule of Beryllium Fluoride. But actually the water molecule H_2O is highly polar and V-shaped. This has been explained by postulating that the oxygen atom O in H_2O water molecule has four orbitals of equivalent energy resulting from SP^3 hybridization (Figure-1 A lower). As shown in Figure-1 B, two of these orbitals contain lone-pair of electrons (from $2s^2$, $2p_x^2$). The other two orbitals have bond-pair electrons, one each from $2p_y^1$ & $2p_z^1$ and another each from two hydrogen atoms (dotted arrows in Figure-1 A, lower).

According to the Valence Shell Electron Pair Repulsion (VSEPR) theory, the lone-pair-lone-pair repulsion is more than the lone-pair-bond-pair repulsion, which in turn is stronger than

the bond-pair-bond-pair repulsion. For maximum stability and minimum potential energy of the molecule these four orbitals orient themselves in a tetrahedral shape (Figure-1 C). For the methane CH_4 molecule, all four orbitals have bond-pair electrons and hence are directed towards the four corners of a *regular tetrahedron*, with a bond angle of 109.5°. Ammonia NH_3 molecule has one lone-pair orbital and three bond-pair orbitals resulting from the SP^3 hybridization for the Nitrogen atom ($1s^2\ 2s^2\ 2p_x^1\ 2p_y^1\ 2p_z^1$ ground state). Shape of the NH_3 molecule is distorted from a regular tetrahedron to a *pyramid* in which nitrogen atom is at the centre, three hydrogen atoms are on the base and lone pair electron at the apex. The bond angle is 107°. [2]

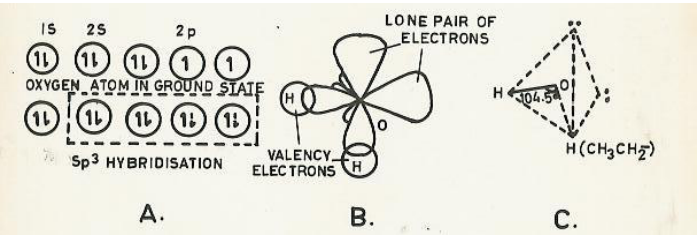

Fig. 1. Tetrahedral (V-shaped) molecule of water formed from SP^3 hybridization of oxygen electrons yielding four equivalent orbitals of which two have lone-pair electrons and the other two have bond-pair electrons. Dotted arrows are electrons from hydrogen H atoms. In ethyl alcohol, one H atom of water is replaced by CH_3CH_2- group

The oxygen atom O in water molecule H_2O has two lone-pair orbitals and two bond-pair ones. It therefore is still more distorted than Ammonia molecule NH_3 to give a bond angle of 104.5° O and a V-shape to the molecule (Figure-1 C). In ethyl alcohol molecule, one hydrogen H of H_2O molecule is replaced by CH_3CH_2- radical (Figure-1 C). The lone-pair orbital is the region of high electron density and a source of electron for electron-seeking atoms and molecules. On the other hand the bond-pair valence electron orbitals are the seats of relative electropositivity, ready to accept electrons. This makes H_2O a polar molecule with a dipole moment of 1.85 Debye, NH_3 of 1.46 Debye and CH_4 none.

4. Energy Levels of Lone-Pair & Bond-Pair Valence Electrons

When the bond-pair valence electron is raised above its ground state of energy E_1 to E_2 it almost immediately i.e. within a pico (10^{-12}) to micro (10^{-6}) sec returns to the ground state and emits a photon of energy $\Delta E = E_2 - E_1 = nh$, where h is the Planck constant and n the frequency of the electromagnetic radiation. The life Δt of the excited state is related to the excitation energy ΔE through the uncertainty relation $\Delta E \cdot \Delta t \geq \hbar$.

The ground state with lowest energy has maximum stability. The difference in adjacent energy levels is largest near the ground state and decreases for higher levels. Therefore the energy levels for the bond-pair valency electron are unevenly and widely separated (Figure 2). The ΔE magnitudes are large and Δt small, of the order of 10^{-6} to 10^{-12} sec. Therefore all excited energy states are unstable.

The lone-pair electron has no definite higher energy orbitals to go to, and is free to be raised or promoted to any higher energy state. Energy levels of the lone-pair electron are therefore closely and evenly spaced (Figure-2, left). From the equation $\Delta E \cdot \Delta t \geq \hbar$, it follows that since the magnitudes of energy difference ΔE between adjacent levels are small the life times Δt of the promoted state are long and therefore the promoted states are long lived.

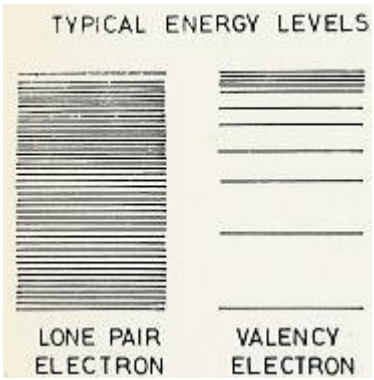

Fig. 2. Energy levels of lone-pair electron and bond-pair valence electron

5. The Electrolysis of Water and Resulting Gas-Mixture

The flow of negatively charged electrons constitutes an electric current. During electrolysis of water under the externally applied electric current the electrons flow from the cathode to the anode inside the electrolyte and from anode to cathode in the external circuit. The water molecule H_2O splits into the cation H^+ and anion OH^-. At the cathode the cation H^+ is *reduced* or neutralized by the incoming electrons e^- to liberate mono-atomic (H) and diatomic (H_2) Hydrogen gas: $2H^+ + 2e^- = 2H = H_2$. At the anode, however, the hydroxyl anion ^-OH is *oxidized* to liberate mono-atomic (O) and diatomic (O_2) oxygen gas and water (H_2O) vapor plus electrons (e^-) which are transported to the cathode via the external circuit: $4OH^- = 2O\ (=O_2) + H_2O + 4e^-$.

5.1. Electrical Promotion of the Lone-Pair Electrons of Oxygen

Above is the usually accepted classical description of the water-electrolysis but it cannot explain the unusual properties of the evolved gas-mixture, which in a way defy explanation by the current Chemistry. The lone-pair and bond-pair electrons (Sec. 3) and their energy levels (Sec. 4) discussed above inescapably force the suggestion that the oxygen atoms in the oxygen gas (O, O_2) and water (H_2O) vapor get promoted to higher energy levels via the electrical energy of electrolysis. This increases the *latent heat of combustion* of the evolved gas-mixture.

5.2. Explanation of the Unusual Characteristics of Evolved Gas-Mixture

This gas-mixture is known to produce a relatively cool flame at 130°C (266°F). Yet it is able to melt metals like steel etc. [1] This can be ascribed to its high *heat of combustion* arising from the long-lived promotion to higher energy levels of the lone-pair electrons of oxygen atoms in the oxygen (O, O_2) gas and water (H_2O) vapor. The gas-mixture is known to burn in vacuum. It happens because it does not need any outside oxygen for its combustion. The gas torch heats but does not boil liquid water, because its water (H_2O) vapor component quietly dissolves in

water un-burnt without generating requisite heat for boiling. But the liquid water in a container boils if the gas flame is directed to heat the container from outside to generate enough heat, as actually observed. [1] It may therefore be concluded that long-lived promotion of lone-pair electrons of oxygen atoms in the gas-mixture provides a plausible, natural theory to explain its unusual characteristics, which otherwise seem to defy explanation within the scope of current theories of Chemistry. No other theory, past or present, is so naturally explanatory.

Acknowledgement

I deeply thank Chris Eckman for arousing my interest in the unusual characteristics of water-electrolysis gas-mixture and for his help and comments for this paper.

References

[1] Chris Eckman, "Characterizing Brown's Gas", Natural Philosophy Alliance Videoconference (9 Dec 2009). http://www.worldsci.org/php/index.php?tab0=Events&tab1=Display&id=253

[2] B. R. Puri and L. R. Sharma, **Principles of Physical Chemistry**, (Vishal Publications, Jullunder, India, 1980).