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PICO-CHEMISTRY: THE POSSIBILITY OF NEW PHASES IN SOME HYDROGEN/METAL SYSTEMS

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In the standard model, matter is an assembly of quarks that combine under the action of the strong nuclear force to give nucleons (protons and neutrons), further giving atom nuclei that under the action of the electromagnetic force combine with electrons to render atoms and molecules. Each of these interactions has a well defined range of binding energies. A novel type of purely electromagnetic interaction is proposed, with binding energies and dimensions between chemistry and nuclear. This type of binding could result in completely novel materials (super-conductivity) and potential energy production.

Keywords: Very strong chemical binding; super-conductivity; energy production.

1. Introduction

The interaction of Hydrogen with certain metals able to absorb or adsorb H (which will be called *A* metals in the text), has been extensively studied, in the view of various applications: Hydrogen storage or Hydrogen isotopes separation,¹ production of finely divided Nickel particles,² room temperature super-conductors,³ etc. The enthalpy of Hydrogen absorption into the *A* metal (hydride formation) or adsorption on the metal surface has been measured and found to be typically in the range 30 to 300 kJ/mole (depending upon the metal or metal alloy used). Recent results obtained with the system Nickel/Hydrogen, under very specific conditions, point to enthalpies of reaction higher than 10 MJ/mole (105 eV/atom), well above the usual values of known chemistry (a few eV). In order to explain these results within the frame of the standard model, the hypothesis of a purely electromagnetic

binding between the Hydrogen and the metal nucleus, which was proposed to be called Pico-Chemistry, has been presented.⁴ A description of the main features of the possible compounds formed at picometer distance between an atom A nucleus, a proton and an electron is given. It is proposed to call these predicted compounds the “Pico-chemistry conjecture”.

2. Requirements for a Pico-Chemical Compound to be Formed

Chemical compounds typically have angstrom size and eV binding electrostatic energies (outer electronic shell). Inside an atom, energies up to more than 100 keV can be found for electrons of the inner shells, but these electrons cannot be involved in any chemical binding: no atom or positive nucleon can reach them because of two barriers: Lenard–Jones potential (related to the Pauli exclusion principle) for an atom and repulsive Coulomb potential for a positive nucleon. Trying to figure out what might be a chemical compound between Hydrogen and a metal, with the level of binding energy that can be found in the inner electronic shell of the metal, requires these two obstacles to be overcome.

3. Possible Formation of a Proton–Electron Dipole

An electrical dipole, formed between an electron and a proton, could meet the above two requirements and thus penetrate into the inner electronic shells of the metal. Should it be possible, this formation must occur under very specific conditions.

A set of experimental conditions has been proposed,⁵ under which the combination of an electron and a proton might result in the formation of a dipole: Ni (that has 4.5 eV work function) and more generally A metals, can be conveniently finely dispersed on calcium oxide (that has a work function lower than 3 eV) using state of the art wet chemical precipitation methods. The resulting catalyst type powder (after NiO reduction by H) can be viewed as nano-size Ni particles randomly resting on an irregular and chaotic CaO surface. The number of Ni atoms in a nano-size particle can be estimated to be several hundreds. At this scale, the border of a Ni particle is not at a constant electrical potential. If H is adsorbed on this surface, it is likely that the positive potential of the proton trapped onto the Ni surface lattice can be felt at several nano-meters from this surface.

When the powder is submitted to a high temperature (500°C) and is a subject to a high Hydrogen pressure (tens of bars), the number of electrons in CaO, having an energy higher than the Fermi level, increases on the one hand and the Ni surface adsorbs H, resulting in protons trapped in its lattice, on the other hand. It is conceivable that higher than Fermi energy electrons from the CaO can be attracted by a proton trapped at the surface of the Ni lattice, overshoot this proton and penetrate into the inner electronic shells of the Nickel. A dipole (hypole \mathbf{H}_A) with a sizeable charge separation is thus formed between the proton and the electron and is attracted by the positive nucleus of the Ni (A metal in general). In order to describe the progression of the dipole towards this nucleus and estimate the possibility of

a bound state (pico-hydride $A\mathbf{H}_A$), the dipole is modeled as a polarized oscillator, the electron oscillating round the proton, with the center of gravity of the electron cloud closer to the Nickel (A metal) nucleus than the proton is. The hypole further reacts with the A metal nucleus to yield the pico-hydride. The characteristics (size and energy of these entities) will be estimated by using the Bohr parameters (radius and energy) that correctly estimate the balance between them.⁶

4. Model for the Polarized Oscillator (Hypole \mathbf{H}_A)

4.1. *The oscillator*

To get the description of the polarized oscillator, the projection of the electron trajectory in the Bohr model of the H atom, on an axis Ni nucleus center/proton center, is considered. In this representation, the electron oscillate round the proton with a frequency $f = v/2\pi r = (1/2\pi)(\mu_e e^4/h^3)$ (v being the velocity of the electron), corresponding to a pulsation $\varpi = \mu_e e^4/h^3 = \sqrt{\kappa/\mu_e}$ (κ = oscillator constant, μ_e electron reduced mass). The binding energy of the electron in the oscillator results from the equation of dynamic $\mu_e(\partial^2 r/\partial t^2 = -(\partial E/\partial r) = -\kappa r$ (κ oscillator constant) and is thus $(1/2)\kappa r^2 = (\mu_e e^4/2h^2) = E_I$ (hydrogen ionization energy). Its size is $r = r_{\mathbf{H}_A} = a_0$ (Bohr radius). The oscillator can have a tangential component (if the electron's motion is not purely radial). This component is neglected but is important and could be modeled the same way as the radial component.

4.2. *The polarized oscillator*

As defined above, the oscillator is not a dipole. Under the influence of the nucleus of A , the oscillator is polarized: the center of gravity of the electron trajectories is at a distance d from the proton, between the A nucleus and the proton. The attractive potential of this center of gravity by the A metal nucleus is $Z e^2/R$, $R = R_{A\mathbf{H}_A}$ being the distance between this center of gravity and the nucleus of A and the attractive potential of it by the proton of the dipole (hypole) is e^2/d . The hypole is stable if: $2(Z e^2/R) \leq (e^2/d)$ or $d \leq (R/2Z)$.

The distance d varies with R , and can be written as $d = kR(1 + \alpha_1 R + \alpha_2 R^2 + \dots + \alpha_n R^n + \dots)$, because at the contact proton/ A nucleus ($R = 0$) the polarization of the electron cloud of the hypole vanishes and $d = 0$. Thus, at first order, $d = kR$. the stability condition is:

$$k \leq \frac{1}{2Z} \tag{1}$$

and the potential between the hypole and A is:

$$V = -Z e^2 \left(\frac{1}{R} - \frac{1}{R+d} \right) \cong -Z e^2 \frac{d}{R^2} \cong -Z e^2 \frac{k}{R}.$$

4.3. Interaction of the polarized oscillator with the atom A

During its progression towards the nucleus of A, the extension r of the hypole will be modified by the interaction of its electron with the nucleus and the electrons of A. At short distance from A (**K** layer radius of A) the problem to solve would be a five particles problem: the A nucleus and its 2 **K** electrons on the one side and the proton and the electron of the hypole on the other side. At this stage, a complete and accurate quantum mechanical treatment of this complex system (if possible) is neither necessary nor justified. **It is thus conjectured** that the hypole electron is submitted to a pseudo central Coulomb potential v from the hypole proton, with an effective charge number K modeling the influence of the A nucleus and its 2 **K** electrons that repel the electron of the hypole with an energy equal to the A metal **K** level energy (Pauli exclusion principle).

Hence: $v = -(Ke^2/r)$ with the limiting condition:

$$K \leq Z + 1. \quad (2)$$

5. Description of the Pico-Hydride and Its Formation

A two step process is considered where the hypole after its formation further reacts with the A nucleus.

5.1. Characteristics of the hypole (\mathbf{H}_A)

The \mathbf{H}_A Bohr radius is:

$$r_{\mathbf{H}_A} = r = \frac{\hbar^2}{\mu_e K e^2} = \frac{a_0}{K} \quad (3)$$

and its energy of formation:

$$E_{\mathbf{H}_A} = \frac{\mu_e K^2 e^4}{2\hbar^2} = K^2 E_I. \quad (4)$$

E_I (13.6 eV) being the ionization energy of the hydrogen atom, a_0 (52.92 pm) the Bohr radius of the H atom and μ_e the reduced mass of the electron in the system proton/electron.

5.2. Characteristics of the pico-hydride (\mathbf{AH}_A)

The pico-hydride has a spherical symmetry centered on the A nucleus: the proton of the hypole rotates round the A nucleus, while its electron oscillates around it. Neglecting the mass of the hypole electron, the \mathbf{AH}_A Bohr radius is:

$$R_{\mathbf{AH}} = R = \frac{\hbar^2}{\mu_H k Z e^2} = \frac{\mu_e}{\mu_H} \frac{1}{k} \frac{a_0}{Z} \quad (5)$$

and its energy of formation:

$$E_{\mathbf{AH}_A} = \frac{\mu_e k^2 Z^2 e^4 \mu_H}{2\hbar^2 \mu_e} = k^2 Z^2 \frac{\mu_H}{\mu_e} E_I \quad (6)$$

from the hypole and the A nucleus (μ_H is the reduced mass of the proton in the system proton/ A metal).

5.3. *Energy of formation of the pico-hydride from the proton, the electron and the A atom*

The total energy of formation of the pico-hydride from its elements is thus:

$$E_T = E_{\mathbf{H}_A} + E_{A\mathbf{H}_A} = \left(K^2 + \frac{\mu_H}{\mu_e} Z^2 k^2 \right) E_I = \left(\frac{K^2}{Z^2} + \frac{\mu_H}{\mu_e} k^2 \right) Z^2 E_I \quad (7)$$

and its dimensions:

$$r_{\mathbf{H}_A} = r = \frac{a_0}{K} \quad \text{and} \quad R_{A\mathbf{H}} = R = \frac{\mu_e}{\mu_H} \frac{1}{k} \frac{a_0}{Z} \quad (8)$$

with the conditions:

$$K \leq Z + 1 \quad \text{and} \quad k \leq \frac{1}{2Z}. \quad (9)$$

The values of the two parameters: k (charge separation factor of the hypole) and K (effective charge number), result from the limit of the progression of the hypole towards the A nucleus, hence:

6. The Pico-Chemistry Conjecture

6.1. *Interaction of the pico-hydride with the electronic layers of A*

The electrons of A have well defined energy levels. Each of these levels is related to the ionization energies of the atom but not equal to, due to the complex interactions between the electrons of the various layers. The Bohr energy of the \mathbf{K} layer is $Z^2 E_I$ and its Bohr radius a_0/Z . The \mathbf{K} layer of the A atom is a limit for the hypole to progress towards the A nucleus. Beyond this limit, the s electrons of A are attracting back the proton of the hypole, which anyhow could not progress more towards the nucleus of A : the dissymmetry of the A atom nucleus + the hypole proton would then vanish and the driving force is reduced to 0. The Bohr radius of the \mathbf{K} electron of A is thus the optimum position of the pico-hydride and can be considered as its ground state (the $\mathbf{L I}$ layer of A would then appear as the first excited state of this pico-hydride, further progression towards the ground state being possible in that case).

Equation (8) results in $R_{A\mathbf{H}} = R = a_0/Z$ (Bohr radius of the A metal \mathbf{K} layer). for $k = \mu_e/\mu_H < 1/2Z$ In that case, choosing $K = Z$ as a first approximation results in $r = R = a_0/Z$. The energy of formation of the pico-hydride is then $E_T = E_{\mathbf{H}_A} + E_{A\mathbf{H}_A} = (1 + \mu_e/\mu_H)Z^2 E_I$. which is the sum of the energy level of the \mathbf{K} layer of A and a small corrective term. For Nickel, $\mu_H/\mu_e = 1.81 * 10^3$. The value of the corrective term is 5.89 eV.

Figure 1 below is a drawing of the pico-hydride, showing the modeled electron trajectory and what might be the real one.

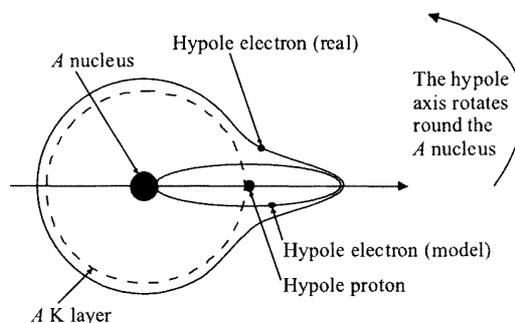


Fig. 1. Schematic drawing of a pico-hydride.

The pico-hydride is thus described as a five particle compound (the nucleus of the atom A and its $2\mathbf{K}$ electrons, and a couple proton/electron, the hypole \mathbf{H}_A). Its stability is achieved by the dissymmetry of the two positive charges inducing a dipolar attraction between them. The localization of the oscillating electron of the hypole is constrained by the \mathbf{K} electrons of the atom A . The axis A nucleus/hypole proton rotates round A .

6.2. The pico-chemistry conjecture

In an environment where protons are trapped in the lattice of a metal A and where free electrons are available, a purely electromagnetic compound of pico-meter size can be formed between the nucleus of A (and its \mathbf{K} electrons), a proton trapped in the lattice of A and a free electron. This compound is proposed to be called A pico-hydride.

The energy of formation of the A pico-hydride comprises two terms: one of the order of magnitude of the \mathbf{K} energy level of A and a second smaller term (ratio μ_e/μ_H). The exact value of the first term will result from the experimental value of K , which will determine the exact extension of the Hypole.

The energy of the excited states of the pico-hydride would depend on and comply with the order of magnitude of the various energy levels of A .

7. Properties of a Pico-Hydride

The best way for characterizing a pico-hydride is to measure its mass. In the case of nickel, certain masses are expected (Table 1), that take into account the energy of formation.

The mass differences given by Table 1, could be easily detected using a high resolution TOF mass spectrometer on an acidic solution of the nickel pico-hydride (probably possible see below, chemical properties). SIMS TOF mass spectrometry is not adapted, since the primary ions energies are of the order of the energy of formation of the pico-hydride. An ICP TOF mass spectrometer would be adapted.

Table 1. Expected masses of nickel pico-hydrides.

Ni parent composition x_i	Ni parent nucleus	Mass parent Ni nucleus	Mass Nickel pico-hydride	Mass of closest stable atom	Closest stable atom	Mass difference ppm
0.68007	58Ni	57.935346	58.943152	58.933198	59Co	169
0.26223	60Ni	59.930788	60.938594	60.931058	61Ni	124
0.0114	61Ni	60.931058	61.938864	61.928346	62Ni	170
0.03634	62Ni	61.928346	62.936152	62.929598	63Cu	104
0.00926	64Ni	63.927968	64.935774	64.927793	65Cu	123

The modifications of the electronic shell of the atom A (Nickel in this case) could be evidenced using EDS-X analysis.

Regarding the chemical properties of NiH_{Ni} , they should be comparable but not identical to the ones of Ni. The outer electronic layers of NiH_{Ni} indeed see the positive charge of the Ni atom, but the structure of these layers could be deeply modified by the pico-hydride presence close to the A nucleus. A modification of the characteristic rays given by Ni in ICP-AOS could be observed. Strong modifications of the physical properties of the Ni (melting point, conductivity and super-conductivity ...) are also expected.

Finally, a very high level of energy should be released during the synthesis of a pico-hydride. No radiations, apart from the predicted weak X-Ray photons occurring during its formation, are expected. A pico-hydride should be stable, because the proton never reaches the Ni (A metal) nucleus. Hence, no radioactive waste is thus expected after a pico-hydride synthesis.

8. Conclusions

In this paper, a rough description of a possible novel chemical interaction and orders of magnitudes of the main characteristics of this still hypothetical interaction, are given.

It is hoped that this approach will be of help when trying to understand the thermal results obtained in certain Ni/H (or other metal/H) systems. This concept might also be useful to explain the modifications of certain physical properties (lowering of the melting point, room temperature super-conductivity) that have been experimentally observed on metal after treatment with Hydrogen.

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