Atomic and molecular structures of positronium, dipositronium and positronium hydride

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Abstract

The three positron based chemical entities, analogous to hydrogen atom, hydrogen molecule and hydride, are drawing increasing attention in the literature. While a lot is known about the binding energies, not much is known about the radii of the atoms and ions and bond lengths and structures of these exotic entities. This article brings for the first time exact values of these structural properties which are comparable with known data. It is hoped that the results will be of help for a better understanding and further development of the chemistry and physics of these exotic compounds and of their possible role as intermediates in chemical and interfacial processes.

Subject terms: Chemical physics, Physical chemistry, Atomic physics, Nuclear physics, Structural chemistry

Positronium (Ps), dipositronium (Ps_2) and positronium hydride (PsH), based on positron, an antimatter, have drawn considerable interest in recent literature. To cite a few, see.[1-8] Several years ago, the author had proposed[9] that, since a neutron (n^0) and a proton (p^+) decay by emitting an electron (e^-) and a positron (e^+) respectively, an ($e^+ e^-$) pair, now known as positronium, could be the intermediate when neutrons and protons fuse together to form atomic nuclei. At distances (a_{e-e+}) of the order of 10^{-15}m, the ($e^- e^+$) pair annihilates releasing two gamma photons of energy, $m_e c^2$ = 0.511 Mev each. This article brings for the first time the structures of the above exotic chemical entities based on exact atomic radii. It is hoped that the results will be of help for a better understanding and further development of the chemistry and physics of these short lived compounds and of their possible yet undiscovered important role as intermediates in chemical and interfacial processes, nucleosynthesis, and biophysics.

Positronium atom,[1-8] is a positron (e^+) bound to an electron (e^-) at a distance of the order of 10^{-10} m as in a hydrogen atom, H in which a proton (p^+) is bound to an electron (e^-) at the distance of the Bohr radius, a_H (~ 0.5 x 10^{-10} m). Dipositronium (Ps_2) is a molecule consisting of a pair of positronium atoms,[3,6] like H_2 where a pair of (p^+e^-) combine to form the molecular hydrogen. Positronium hydride (PsH) is a diatomic molecule,[4,6,7] which can be completely or partially covalent or ionic. Considered here are the ionization energy, Bohr radius and bond lengths in the above, based on exact atomic and ionic radii evaluated here for the first time. The observed bond lengths of PsH are comparable with the corresponding sums of the ionic and atomic radii obtained here.

The ionization energy, Bohr radius and reduced mass relation for Ps can be considered similar[1a,10] to that for H. The ground state energy, $E_H = eI_H$ (where I_H is the ionization potential and e is the elementary charge), Bohr radius, a_H (which is the distance between the electron and proton) and the reduced mass, $\mu_{H,red} = m_{e-}m_{p+}/(m_{e-} + m_{p+})$ (where m_{e-} and m_{p+} are masses of the electron and proton respectively), are related as follows,[11,12]

$$E_H = (1/2)(e^2/\kappa a_H) = (1/2)\mu_{H,red}(\alpha c)^2 = eI_H \qquad (1a\text{-}c)$$

where, $\kappa = 4\pi\varepsilon_0$, the atomic unit of permittivity, ε_0, the electric constant, α, the fine structure constant, h, the Planck constant and c, the speed of light in vacuum. On using the latest values,[13] of the physical constants, it follows that

$$\mu_{H,red} = 0.910442 \times 10^{-31}\text{ kg} \qquad (2)$$

$$E_H = (1/2)\mu_{H,red}(\alpha c)^2 = 2.178686 \times 10^{-18}\text{ J} \qquad (3)$$

$$I_H = E_H/e = 13.5983\text{ V} \qquad (4)$$

$$a_H = (1/2)(e/\kappa I_H) = 0.5295 \times 10^{-10}\text{m} = 0.05295\text{ nm.} \qquad (5)$$

Bohr radius (a_H) was shown to be the sum of two Golden sections $a_{H,e-}$ and $a_{H,p+}$ pertaining to the electron and proton[11,12]: In equation (1c), $I_H = (I_{p+} + I_{e-})/2$ where $I_p = e/(\kappa a_{H,p+})$ and $I_{e-} = -e/(\kappa a_{H,e-})$ are the components of the ionization potential, and $a_{H,e-}$ and $a_{H,p+}$, are sections of a_H pertaining to (p^+) and (e^-) respectively. Thus,

$$I_H = (1/2)(e/\kappa a_H) = (1/2)(e/\kappa)[(1/a_{H,p+}) - (1/a_{H,e-})] \qquad (6a,b)$$

$$1/a_H = (1/a_{H,p+}) - (1/a_{H,e-});\ a_H = a_{H,e-} + a_{H,p+} \qquad (7a,b)$$

$$(a_{H,e-}/a_{H,p+})^2 - (a_{H,e-}/a_{H,p+}) = 1 \qquad (8)$$

On combining equations (7a & b), one obtains equation (8), which is a Golden quadratic equation, whose positive root is $a_{H,e-}/a_{H,p+} = \varphi = (5^{1/2} + 1)/2 = 1.618034..$, the Golden ratio, a mathematical constant.[14] This shows Nature's unique construction of the atom, that a_H is divided at the Golden point at the point of electrical neutrality P_{el}, into the two Golden sections $a_{H,e-}$ and $a_{H,p+}$ pertaining to the electron and proton. These Golden sections are given by,

$$a_{H,e-} = a_H/\varphi = 0.3272 \times 10^{-10}\text{m};\ a_{H,p+} = a_H/\varphi^2 = a_{H,e-}/\varphi = 0.2022 \times 10^{-10}\text{m} \qquad (9a,b)$$

Figure 1a shows the hydrogen atom, with the two circles of radii $a_{H,e-}$ and $a_{H,p+}$ pertaining to the electron and proton.

In the case of positronium, Ps, which consists of an electron and a positron, equations similar to those for H hold, but with the reduced mass,[1a,10] $\mu_{Ps,red} = m_{e-}/2$,

$$\mu_{Ps,red} = m_{e+}m_{e-}/(m_{e+} + m_{e-}) = m_{e-}/2 = 4.554691 \times 10^{-31}\text{kg}. \qquad (10)$$

$$E_{Ps} = (1/2)\mu_{Ps,red}(\alpha c)^2 = 1.089945 \times 10^{-17}\ \text{J} \qquad (11)$$

$$I_{Ps} = E_{Ps}/e = 6.803\ \text{V} \qquad (12)$$

$$a_{Ps} = (1/2)(e/\kappa I_{Ps}) = 1.0583 \times 10^{-10}\ \text{m} = 0.10583\ \text{nm} \qquad (13)$$

The value of I_{Ps} is the same as that, 6.803 V in.[1a,4,5] and $a_{Ps} \sim 2a_H$. as reported in.[2]

Bohr radius (a_{Ps}) of positronium is likewise the sum of the two Golden sections $a_{Ps,e-}$ and $a_{Ps,e+}$ pertaining to the electron and positron. The Golden sections of a_{Ps} (= $a_{Ps,e+}$ + $a_{Ps,e-}$) give the radii of e^- and e^+ in Ps as in the case of H,

$$a_{Ps,e+} = a_{Ps}/\phi^2 = 0.4042 \text{ x } 10^{-10} \text{ m}; \; a_{Ps,e-} = a_{Ps}/\phi = 0.6541 \text{ x } 10^{-10} \text{ m} \qquad (14)$$

Figure 2a shows the positronium with the two circles of radii $a_{Ps,e-}$ and $a_{Ps,e+}$ pertaining to the electron and positron.

As in the case of the hydrogen molecule, H_2, where a proton and an electron occupy the opposite corners[11,12] (see Figure 1b) of a square, dipositronium, Ps_2, can be considered as a square with an electron and positron on opposite corners as in Figure 2b. The length of the covalent bond in the H_2 molecule, d(H-H), (see Figure 1c) is equal to the diagonal of the square with the Bohr radius, $a_{B,H}$ as a side[11] and the covalent radius,[15] R_H = d(H-H)/2, as given by,

$$d(H\text{-}H) = 2^{1/2}a_{B,H} = 0.07488 \text{ nm} \qquad (15)$$

$$R_H = 0.03744 \text{ nm} \qquad (16)$$

The Golden sections of d(H-H) give the cationic and anionic radii[11,12] of the ionic resonance forms[15] of H_2 (see Figure 1d)

$$d(H\text{-}H) = d(H^+) + d(H^-) = 0.07488 \text{ nm} \qquad (17)$$

$$d(H^+) = d(H\text{-}H)/\phi^2 = 2^{1/2}a_{H,e+} = 0.02860 \text{ nm} \qquad (18)$$

$d(H^-) = d(H\text{-}H)/\phi = 2^{1/2}a_{H,e-} = 0.04628$ nm (19)

The covalent bond length, d(Ps-Ps) of Ps_2 can similarly be obtained as the diagonal of a square with $a_{B,Ps}$ as the sides (see Figures 2b,c),

$d(Ps\text{-}Ps) = 2^{1/2}a_{B,Ps} = 0.1497$ nm (20)

$R_{Ps} = d(Ps\text{-}Ps)/2 = 0.07485$ nm (21)

where the two electrons and two positrons are at the opposite corners of the square. This bond length (see Figure 2c) is nearly 2d(H-H). The covalent radius, R_{Ps} (see Figure 2c) is comparable with half the diameter, 0.159 nm reported in.[4]

As in the case of hydrogen, the Golden sections of d(Ps-Ps) give the radii of the cation Ps^+ and anion Ps^- (see Figure 2d),

$d(Ps\text{-}Ps) = d(Ps^+) + d(Ps^-) = 0.1497$ nm (22)

$d(Ps^+) = d(Ps\text{-}Ps)/\phi^2 = 2^{1/2}a_{Ps,e+} = 0.0572$ nm (23)

$d(Ps^-) = d(Ps\text{-}Ps)/\phi = 2^{1/2}a_{Ps,e-} = 0.0925$ nm (24)

The bond length of positronium hydride, PsH,[4,6,7] consting of a positronium ion or atom and a hydrogen atom or ion depends on the many possible forms.[7] In,[4] PsH is considered as an atom and not molecule. However, since in PsH there are two distinct positive nuclei (a positron and a proton) sharing the two electrons, here it is considered as a molecule. Four of the possible bond lengths obtained as the sums of the radii are given below (see Figures 3 a -d) as examples:

$$d(Ps^{+}H^{-}) = d(Ps^{+}) + d(H^{-}) = 0.0572 + 0.0462 = 0.103 \text{ nm} \quad (25)$$

$$d(PsH) = d(Ps) + d(H) = 0.075 + 0.037 = 0.112 \text{ nm.} \quad (26)$$

$$d(Ps^{-}H^{+}) = d(Ps^{-}) + d(H^{+}) = 0.0925 + 0.0286 = 0.121 \text{ nm.} \quad (27)$$

$$d(Ps^{-}H^{-}) = d(Ps^{-}) + d(H^{-}) = 0.0925 + 0.0462 = 0.139 \text{ nm} \quad (28)$$

In the above, $(Ps^{+}H^{-})$, $(Ps^{-}H^{+})$ and $(Ps^{-}H^{-})$ are completely ionic bonds and PsH is a completely covalent bond. The bond length $d(Ps^{-}H^{+})$ = 0.121 nm in equation (27), is close to the electron-proton distance, $2.31a_{B,H}$ = 0.122 nm in,[6] and that of $d(Ps^{-}H^{-})$ of equation (28) corresponds to the positron-proton distance, 0.14 nm in.[7] For a comparison of the above bond lengths with those of many hydrides, see.[16-18]

Summary

This work presents for the first time exact values of the radii, bond lengths, dimensions and structures of positronium, dipositronium and positronium hydride at the atomic level and it is hoped that this will be of fundamental help in the study of these exotic atoms and molecules consisting of antimatter and their possible role as important short lived intermediates in chemical, biochemical and nuclear processes

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Competing financial interests

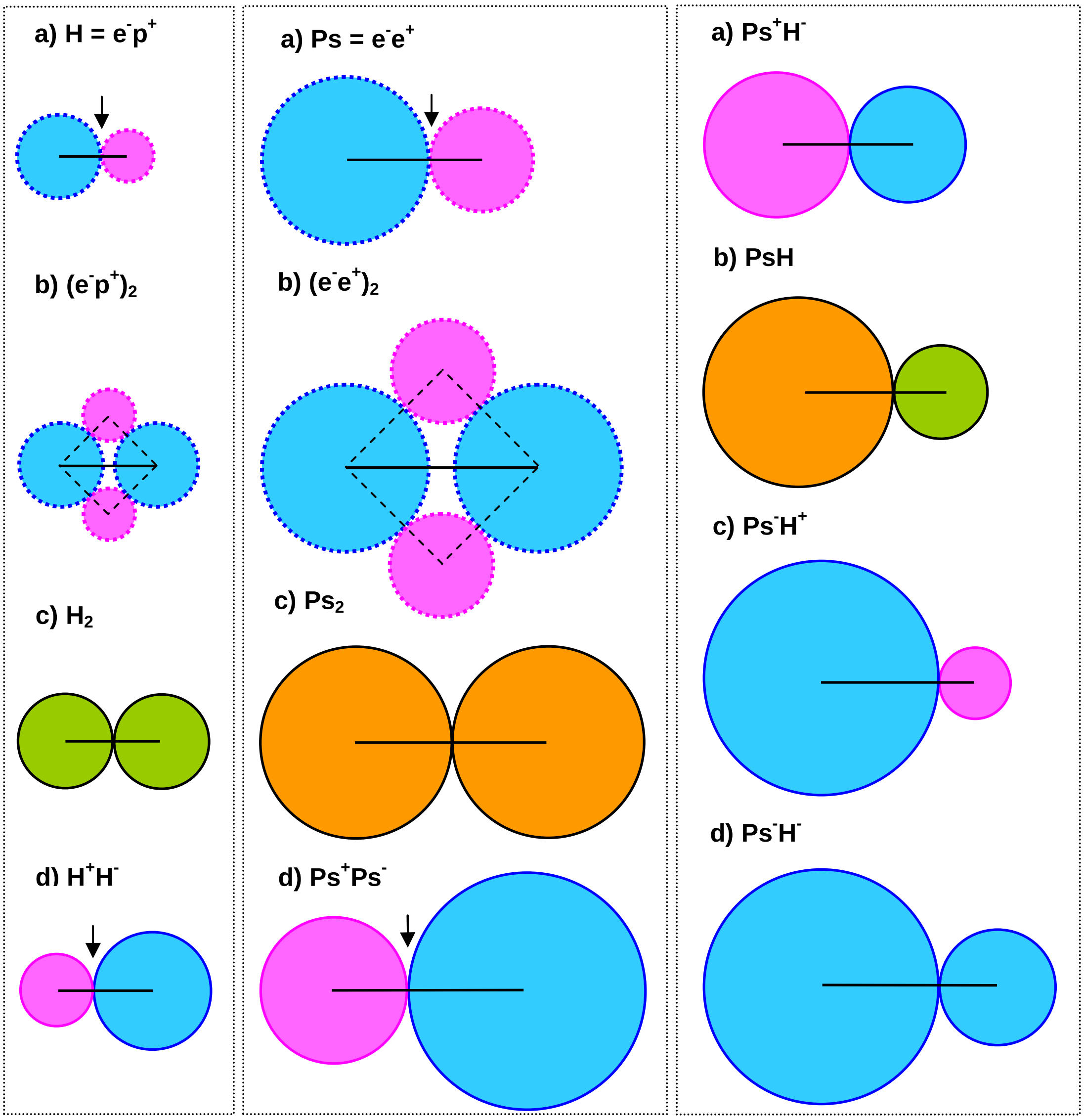
There are no competing financial interests

Legends for Figures.

Figure 1. Hydrogen (H). a) H = e^-p^+; separated by Bohr radius (a_H). The blue and pink circles have the radii, $a_{H,e-}$ and $a_{H,p+}$ respectively and the Golden point (point of electrical neutrality, P_{el}) is marked by the arrow, b) a pair of (e^-p^+) forming H_2, as a square of side a_H, c) H_2 molecule with bond length d(H-H) = $2^{1/2}a_H$ and d) d(H-H) = d(H^-) + d(H^+). The blue and pink circles have the radii d(H^-) and d(H^+) respectively, and the Golden point is marked by the arrow.

Figure 2. Positronium (Ps). a) Ps = e^-e^+; separated by Bohr radius ($a_{Ps} \sim 2a_H$). The blue and pink circles have the radii, $a_{Ps,e-}$ and $a_{Ps,e+}$ respectively and the Golden point (point of electrical neutrality, P_{el}) is marked by the arrow, b) a pair of (e^-e^+) forming Ps_2, as a square of side a_{Ps}, c) Ps_2 molecule with bond length d(Ps-Ps) = $2^{1/2}$ a_{Ps} and d) d(Ps-Ps) = d(Ps^-) + d(Ps^+). The blue and pink circles have the radii d(Ps^-) and d(Ps^+) respectively, and the Golden point is marked by the arrow.

Figure 3. Positronium hydride. a) Ps^+H^-, b) PsH and c) Ps^-H^+, where the cation Ps^+ and anion Ps^- are from Fig. 2d and the cation, H^+ and anion, H^- are from Fig. 1d. The bond lengths are sums of the radii of the adjacent atoms or ions: a) d(Ps^+H^-) = 0.103 nm, b) d(PsH) = 0.112 nm. c) d(Ps^-H^+) = 0.121 nm and d) d(Ps^-H^-) = 0.139 nm.



Figures 1 - 3